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TECHNICAL REPORT 9302

THE POLLUTANT HAZARD ASSESSMENT SYSTEM

VERSION 3: DOCUMENTATION AND USERS MANUAL

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MAY 1993

U S ARMY BIOMEDICAL RESEARCH & DEVELOPMENT LABORATORY

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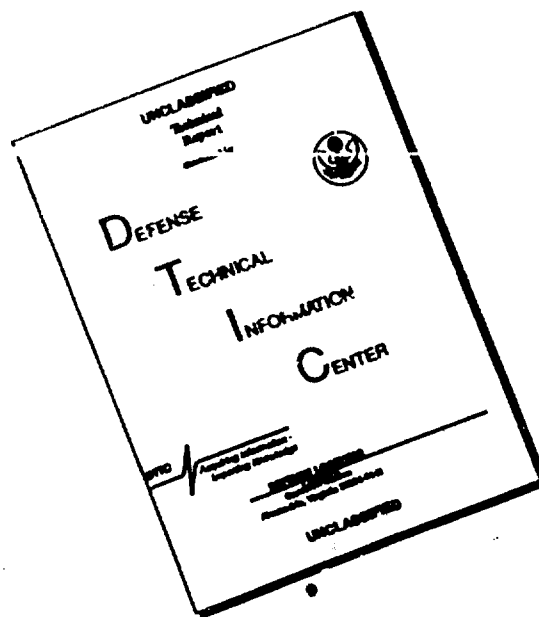
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19. ABSTRACT (Continue on reverse if necessary and identify by block number) This report describes a comprehensive revision of software described in Technical Report 9104 (The Pollution Hazard Assessment System Version 20: Documentation and Users Manual) which was issued in March 1991. The revised software, referred to as PHAS3, is programmed in BASIC code. The system is sufficiently compact to be handled on most personal computer configurations, and can be supported with a computer with 640K memory, a monochrome monitor, and a line printer. The revision incorporates several improvements made in programs after the issue of Technical Report 9104 that were described in an addendum/errata issued by the author, improves the assessment of hazardous sites with respect to area and depth of contamination, and provides for in-situ transformation of contaminant due to environmental processes.					
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PHAS3 is designed for general use in risk assessments, such as the "baseline assessment" detailed in the most recent Risk Assessment Guidance for Superfund (EPA/540/1-89/002). PHAS3 performs the risk assessment on the basis of a "unit concentration" algorithm and provides outputs from which hazard indices can be developed. The algorithm is compatible with those described in the Guidance, but provides more generalized results so as to be more universal in application. PHAS3 lets the user incorporate information about potential effects to indigenous biota in the environment so that the assessment encompasses both human and biota implications.

PHAS3 guides the user through the system with instructional menu displays provided for specific tasks of data and information processing, modification, and storage. The user can prepare information or data for immediate analysis or store information in off-line files for recall. These files can be rapidly downloaded for system use. Three sets of user files are employed: files that store information about scenario exposure pathways; files that store non-chemical data (i.e.: human intake rates, site-specific soil and drainage parameters, time scales, and for meat or dairy intake, livestock characteristics); and files that store chemical-related data (i.e.: physicochemical properties, transfer or partition coefficients, in-situ transformation rate constants, Public Health toxicity information, and environmental biota limits). The exposure pathways presented cover many common water, fish, vegetable, meat or dairy intake situations, as well as (for soil) direct exposure intakes and diffused vapor dispersed in air situations. PHAS3 contains a chemical-related data estimation subroutine package. This package can be accessed from data processing routines directly for the purpose of developing online data for analyses or storage. The package can be also accessed in a "desk-calculator" mode.

The main text provides the user with a discussion of PHAS3 health-effects related concepts and operational instructions. Appendix A presents a glossary of terms and data identifications. Appendix B contains the equations used to describe scenario exposure pathways and other risk assessment analyses.

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## PREFACE

This report documents computer software developed under Work Unit 686 (Hazard Assessment Method Computerization) in the Environmental Quality Research Branch of the Health Effects Research Division.

The author acknowledges the support of Jesse J. Barkley, Jr., Branch Chief. The author thanks Mr. Jeffrey D. Leach of Fort Detrick's Directorate of Information Management for many suggestions provided in the review of the report's draft text and for improvements to the PHAS3 program code. The author also thanks Dr. Howard T. Bausum for his technical review.

The Defense Technical Information Center does not supply software. The author will supply the software to persons who provide either one unmarked two-sided high-density 5-1/4 inch floppy disk or one unmarked 3-1/2 inch diskette. A suitable mailer should also be supplied. Send disks to

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## ADDENDUM

1. Table 2. The dates and file lengths of files provided on your disk may differ from those cited in the Table.

2. "quit" inputs. PHAS3 allows the user to exit without action from routines that require an input or output filename. At the filename prompt, enter "quit". This feature is provided in case the wrong routine was selected and the user is in danger of losing online data or creating an unneeded file. The specific sections involved are listed below; the listing also indicates subsequent displays.

Section 5.3; the PATWAY3 main selection menu appears.

Section 5.5 (PTLD3 input); the PATWAY3 main selection menu appears.

Section 5.6; the PATWAY3 main selection menu appears.

Section 6.2 for an .LDS file input; the NOCH3 main selection menu appears.

Section 6.3; the NOCH3 main menu appears.

Section 7.1 or 7.2 for .DAT file input; the CHMF3 main selection menu appears.

Section 7.3; the CHMF3 main selection menu appears.

Section 11.0; the user is prompted for another .LDS filename.

## CONTENTS

<b>PREFACE</b>	<b>1</b>
<b>1.0 INTRODUCTION</b>	<b>6</b>
<b>2.0 PHAS3 EXPOSURE ASSESSMENT CONCEPTS</b>	<b>6</b>
2.1 Comparison of PHAS3 to EPA Guidance	8
2.2 PHAS3 Treatment of Special Situations	10
2.2.1 Hazardous Land Sites	10
2.2.2 Dermal and Respired Pollutant Intakes	10
2.2.3 Time-Related Terms	12
2.3 PHAS3 Applications	13
2.3.1 Remedial Investigation Planning and Performance	13
2.3.2 Visualization of Public Health Data	14
2.3.3 Integration of Non-Public Health Effects	15
<b>3.0 DESCRIPTION OF PHAS3 STRUCTURE</b>	<b>16</b>
3.1 Hardware	16
3.2 Definitions	16
3.3 System Structure and External Files	16
<b>4.0 PHAS3 INSTALLATION AND START UP</b>	<b>19</b>
4.1 Installing PHAS3	19
4.2 System Notes and Programming Conventions	21
4.3 OPEN3	22
<b>5.0 PATWAY3</b>	<b>24</b>
5.1 Source Medium Selection	24
5.2 Stored Filenames Review	24
5.3 Stored File Downloading	25
5.4 Scenario Creation	25
5.5 The Scenario Data Needs Report	26
5.6 Scenario Information Storage	35
<b>6.0 NOCH3</b>	<b>36</b>
6.1 Download a .LDS File and Return to OPEN3 ("Load and Go")	36
6.2 .LDS File Retrieval, Data Review and Change Procedures	37
6.3 The Data Storage Routine	40
6.4 Data Review and Change Routine For Air Dispersion Terms	41
6.4.1 MXb	41
6.4.2 MXon	43
6.4.3 MXof	43
6.4.4 MXef	44

7.0	CHMF3	48
7.1	Download a .DAT File	48
7.2	.DAT File Retrieval, Data Review and Change Procedures	48
7.3	.DAT File Storage	49
7.4	Modify Online Data via the CRDES3 Selection Menu (function '6')	49
7.5	Chemical-Related Data File Structure	52
8.0	DIAG3	53
8.1	Display Pathway Status (SST) for Online Scenario	53
8.2	Display Data Use Status Table (DUST) for a Scenario	55
8.3	Online Data Displays	56
8.4	Online Data Printouts	57
8.5	Review and Change Online Data	58
9.0	ASSESSMENT AND CONSTRAINT ANALYSIS PROGRAMS	62
9.1	The Public Health Assessment Program, COMP3	62
9.2	The Constraint Analyses Programs CONWS and CONTS	65
10.0	CRDES3	69
10.1	General CRDES3 Access and Exit Procedures	69
10.2	Estimation Method Subroutines Procedures	70
10.3	Estimation Subroutines in CRD013	70
10.3.1	Water Solubility (Wsol)	70
10.3.2	Boiling Point (Tb)	70
10.3.3	Vapor Pressure (VP)	72
10.3.4	Soil Organic Carbon-Water Partition Coefficient (Koc)	75
10.3.5	Soil to Vegetable and Plant Partition Coefficients (Ksv and Ksp)	75
10.3.6	Plant to Adipose Tissue Partition Coefficient (Kpat)	75
10.3.7	Diffusivity in Air (Da)	76
10.3.8	Diffusivity in Water (Dw)	77
10.3.9	Henry's Law Constant (Kh)	78
10.3.10	Dermal Permeability Coefficient (PC)	78
10.3.11	Fish Bioconcentration Factor (BCF)	78
10.3.12	Water to Vegetable and Plant Partition Coefficients (Kwv and Kwp)	78
10.3.13	Fish Bioaccumulation Factor (BAF)	79
11.0	CRD113	80
11.1	Plant to Beef Partition Coefficient (Kpm)	80
11.2	Plant to Milk Partition Coefficient (Kpd)	81
11.3	Soil to Water Partition Coefficient (Kd)	81
11.4	Soil to Surface Water Runoff Coefficients (MKro1 and MKro2)	82
11.5	Soil Flux Partition Coefficients (MKdb and MKdo)	83
11.6	Sediment Flux Partition Coefficient (MKdw)	88
11.7	Groundwater Infiltration Partition Coefficient (MKgw)	90



12.0	REFERENCES	93
12.1	References Cited in Text	93
12.2	References Cited Only in PHAS3 Information Files	95
APPENDIX A.	GLOSSARY OF TERMS, ACRONYMS, AND DATANAMES IN MAIN TEXT	97
APPENDIX B.	PATHWAY AND CONSTRAINT EQUATIONS	103
B.1	Special Terms Used in Equations	103
B.2	Assumptions Implied in Pathway Intake Equations	103
B.3	Water Related Pathways	104
B.4	Surface Soil Related Pathways	106
B.5	Sediment Related Pathways	110
B.6	Type 1 Constraint Equations	111
B.7	Type 2 Constraints	112
B.8	Special Topics	113
B.8.1	EIwa and EIwc Values in DEFAULT.LDS	113
B.8.2	Time-Averaged Functions	114
B.8.3	Derivation of MGPCC for Pathway Equation 11	115
B.8.4	Time Intervals to Estimate MK-Partition Coefficients	115
APPENDIX C.	SPECIAL PHAS3 ERROR TRAPS AND THEIR RESOLUTION	116
C-1	Special Error Traps in OPEN3	116
C-2	Missing File Error Traps	116
DISTRIBUTION		118

### Figures

1.	Unit Intake Curves Illustrating the Impact of Time Dependency	13
2.	Relation of the PPLVs of Two Pollutants to Hazard Index and Type 1 Constraints	15
3.	PHAS3 System Structure and Program-File Relationships	18
4.	Command Sequence to Install PHAS3 as Described in Section 4.1	21
5.	OPEN3 Main Selection Menu	23
6.	Initial Display of the PATWAY3 Main Selection Menu	24
7.	Sections from Sample Problem Pathway Selection and Data Needs Summary Report (3 pages)	28
8.	NOCH3 Main Selection Menu Display	36
9.	Sample Display, NOCH3 Data Review and Change Routine	39
10.	Sample Display and Processing Sequence for MXon in NOCH3	42
11.	WECF Contours by Month	
a.	November through February	45
b.	March through June	46
c.	July through October	47
12.	Initial Display from CHMF3	49
13.	Sample Processing Sequence, CHMF3 Data Review and Change Routine	50
14.	CRDES3 Selection Menu Accessed from CHMF3 via Function '6'	51
15.	DIAG3 Display of SST for PTSAMPLE.PTS	54
16.	DIAG3 Display of DUST for PTSAMPLE.PTS	55

17.	DIAG3 Display of Database in DEFAULT.LDS	56
18.	DIAG3 Display of Database in DEFCEM.DAT	57
19.	DIAG3 Printout of Databases from DEFAULT.LDS and DEFCEM.DAT, Option 3 (two pages)	59
20.	Sample Display of DIAG3 Data Review and Change Routine	61
21.	COMP3 Assessment of Sample Problem	64
22.	COMP3 Assessment of Hypothetical Water-Base Medium Problem	64
23.	Part of Type 1 Constraint Analysis for Sample Problem	66
24.	Type 1 Constraint Analysis, Problem from Figure 22	67
25.	Type 2 Constraint Analysis, Sample Problem.	68
26.	Miller's Boiling Point Method Displays	71
27.	Vapor Pressure Information Message	73
28.	Watson's Vapor Pressure Method Display. CRDES3 Access from OPEN3	73
29.	Koc Estimation Method 2 Display. CRDES3 Access from OPEN3	76
30.	Information Message for Da and LeBas Volume Displays	77
31.	Kpm Subroutine Display with CRDES3-CHMF3 Interface for Mode 2 Access	81
32.	Rain/Runoff Factors for the Eastern United States	84
33.	MKrol Estimation by USLE-Haithe Approach. CRDES3 Access from OPEN3	85
34.	MKdba Estimation in CRD113. CRDES3 Access from OPEN3	86
35.	MKdwa Estimation in CRD113. Access From CHMF3 Under DUST Control	89
36.	MKgwa Estimation in CRD113. CRDES3 Access from OPEN3	91

#### Tables

1.	PHAS3 Exposure Pathways in Order of Presentation	11
2.	Files Supplied on Subdirectory \PHAS3\DISK1	20
3.	Dataname and Symbols Used in PHAS3 (4 pages)	28
4.	Pathway (Route) Location Number for SST Display in DIAG3	53

## 1.0 INTRODUCTION

The Pollution Hazard Assessment System, version 3 (PHAS3) is a suite of programs designed to assist in exposure assessments at known or suspected hazardous waste sites. PHAS3 is designed for use on the IBM Personal Computer, its family of successors, and compatible computers. PHAS3 is a replacement for PHAS Version 20, which was also developed by Small<sup>1</sup>.

This document describes PHAS3. The general exposure assessment problem is discussed in Section 2. This section's discussion is presented to promote an understanding of the PHAS3 treatment of the problem, and that PHAS3 treatment of assessments conform to U.S. Environmental Protection Agency (EPA) Superfund risk assessment guidance<sup>2,3</sup>. The system structure is reviewed in Section 3. Sections 4 through 11 present instructions for use of specific PHAS3 programs, and discuss program printouts and displays. These sections comprise the "user's manual" for PHAS3 and cover the "how to" aspects of PHAS3. The report has three appendices. Appendix A provides a glossary of terms. Appendix B presents and discusses assessment equations used in PHAS3, including assumptions and restrictions. Appendix C discusses error messages.

## 2.0 PHAS3 EXPOSURE ASSESSMENT CONCEPTS

Here, the exposure assessment problem is discussed in generic terms. For purposes of illustration, this discussion will be directed to land contamination. The assessment process involves these steps:

- o Determine pollutants of concern.
- o Define how people will be exposed to the pollutant, i.e. specify component exposure pathways. The aggregate of these pathways is a scenario.
- o Develop an equation (or equations) for each pathway that relates the human intake (or dose) of a substance to the substance concentration in soil.
- o Collect the data needed to solve such equations.
- o For each pollutant and scenario, use the developed equations to compute an intake (or dose) corresponding to some "representative" pollutant concentration in soil.
- o Compare the computed intake (or dose) to some pre-set intake or dose.
- o Interpret the results, and
- o Determine if non-public health considerations, such as aquatic toxicity or phytotoxic effects, might be more restrictive than public health considerations.

Hazardous waste site, and particularly "Superfund" site remediations are an important application of such assessments. In 1989, the EPA issued the Risk Assessment Guidance for Superfund. Volume I-Human Health Evaluation Manual, Part A<sup>2</sup> (RAGS) for the specific application of "developing health risk

information at Superfund sites". RAGS\* and PHAS3 must not be thought of as exclusive or competing alternatives; PHAS3 complies with RAGS, but is designed to be more generalized in its applications. Due to the wide dissemination of RAGS, its sections are cited in subsequent paragraphs of this report.

The first two steps in the assessment process address the questions "What are the contaminants and how are or will people be reasonably expected to be exposed to them?" The contaminants are often tentatively identified from a records study of site operations. For example, at an old explosives production plant, the raw materials, product explosives intermediates, and by-products would be possible contaminants. This study may be augmented by preliminary sampling to identify other contaminants. One could expect that, if production-related substances are peculiar to the site, the substances are contaminants. Sometimes, contaminants have to be distinguished from naturally-occurring or anthropogenic substances in terms of concentration or distribution. Chapter 4 of RAGS discusses this distinction.

In the second step, exposure pathways are defined. A pathway may include more than one specific route by which people can be exposed to a pollutant. For example, assume that a community near a hazardous waste site uses groundwater as a domestic water source. Pollutants from the site can percolate to this groundwater. Assume further that the community has a small recreational lake for water activities, that the lake is also used for fishing, and pollutant in soil from the site may be carried in run-off to this lake. Three exposure pathways can be identified: domestic water exposure, recreational water exposure, and fish intake. However, the first two pathways can each include three exposure routes -- ingestion, dermal absorption, and inhalation (of pollutant vapors released from water). Thus, the scenario (which might be titled "resident exposure near a site") consists of three exposure pathways and seven routes. RAGS further discusses pathways and routes in Chapter 6. PHAS3 includes all pathways and routes discussed in RAGS.

The scenarios may relate to current activities, or those projected in the future during or after remedial actions. Different scenarios may be defined for adults and children in the same area.

For each proposed pathway (or route, when necessary), an equation describes the relation between human intake and the pollutant concentration in soil. Section 6.6 of RAGS presents equations for expected routes. These equations are in the general form:

$$\text{Dose} = \text{Consumption or ingestion rate of item to which humans are exposed} \times \text{Model exchange and transfer from soil to the exposure item} \times \text{Time adjustment factors} \times \text{Pollutant concentration in soil} \quad (1)$$

The pollutant concentration data is obtained from analysis of soil samples. The other data that enters into these equations can be classified into two broad categories. The first of these is non-chemical data, data that would be applicable independent of the chemical involved. This would include data involved in the "consumption or ingestion rate of item to which humans are

\* Several reference in the text and in PHAS3 program files are referred to by acronyms. These acronyms are listed in Appendix A.

exposed" term. In terms of the scenario example, such data would include the consumptive intake of domestic water, the daily intake of fish, or inhalation of air (where pollutant transfers from water to air). Time adjustment factors also are non-chemical data, since they reflect the lifestyle of receptors.

The "model exchange and transfer from soil to the exposure items" can include data that is solely non-chemical (such as wind speed or dispersion terms when routes involve pollutant in air), data that is solely chemical-related (such as fish bioaccumulation factor), or data from both categories. One such term in the scenario example would be the pollutant concentration in water per unit concentration in soil due to runoff. This term would be computed from non-chemical data such as soil condition and cultivation factors, and chemical-related data such as the pollutant's organic carbon (in soil)-water partition coefficient. Such PHAS3 data are called "super" partition coefficients. These coefficients are strictly "mixed"; they are based on non-chemical and chemical-related data. PHAS3 processes them along with chemical-related data.

The interpretation of results depends on the specific problem. For the Superfund risk assessments, RAGS procedure is to divide the sum of doses from each route's intake equation by a public health limit dose (PHLD) to define a pollutant's hazard index. The specific PHLD is associated with an adverse effect to be avoided (a toxic response, a specified increased risk of carcinogenicity, teratogenicity effects, etc.). An example of such a dose would be the EPA Reference Dose (RfD). Here, dose units are mg/kg-day.

The index is summed for all pollutants with similar health effects as discussed in Chapters 7 and 8 of RAGS. If this index is one or less, scenario exposure to the considered pollutants is unlikely to pose a public health concern. In terms of the site situation and the public health standpoint, the site probably is "clean" and needs no remediation.

The conclusion is subject to two constraints. There is no guarantee that a "clean" site would be safe for indigenous species of the ecosystem. They must be considered in a complete analysis. If an untreated site has the potential to cause unacceptable adverse effects to other biota, or aesthetic problems, remediation may be needed regardless of a negligible public health concern. A second constraint is that the physico-chemical properties of a substance, particularly water solubility, may limit its transfer to humans. If the hazard index exceeds one, and this constraint occurs, the assessment must be critically re-examined. In equation 1, there is an implied proportionality between dose and concentration, which may be invalid if this constraint occurs.

## 2.1 Comparison of PHAS3 to EPA Guidance

In the exposure assessment equations presented in RAGS, the term "intake" is used in the context of dose (see RAGS, page 8-2). PHAS3 considers "intake" in terms of mass/day. The conversion is: dose x body weight = mass/day intake. PHAS3 uses a "unit concentration" intake algorithm; in the case of soil contamination, the intake equations are solved in terms of 1 mg pollutant/kg soil. Once the intake is computed, results can be "scaled" for exposure assessment needs.

Exhibit 6-14 in RAGS is an illustrate example. The pathway described is residential exposure to ambient soil with one specific route -- ingestion of soil. The route intake-concentration equation presented is:

$$\text{RAGSTAKE} = \text{CS} \times \text{IR} \times \text{CF} \times \text{FI} \times \text{EF} \times \text{ED} / (\text{BW} \times \text{AT}) \quad (2)$$

RAGSTAKE = daily ingestion of chemical per unit body weight (mg/kg-day)  
 CS = chemical concentration in soil (mg/kg)  
 IR = Ingestion rate (mg soil/day)  
 CF = Conversion factor ( $10^{-6}$  kg/mg)  
 FI = Fraction of soil ingested from contaminated soil (unitless)  
 EF = Exposure frequency (days/years)  
 ED = Exposure duration (years)  
 BW = Body weight (kg)  
 AT = Averaging time (time over which exposure is averaged-days)

The product RAGSTAKE x BW is an intake in mg/day; dividing this intake by CS provides a daily intake for 1 mg/kg chemical in soil. The term IR x CF x FI can be combined into one term, the kg/day of contaminated soil ingested. The term EF x ED / AT is a time adjustment factor (see equation 1); it converts a daily soil ingestion situation into the specific intake situation hypothesized for the scenario. Equation 2 can be regrouped:

$$(\text{RAGSTAKE} \times \text{BW} / \text{CS}) = (\text{IR} \times \text{CF} \times \text{FI}) \times (\text{EF} \times \text{ED} / \text{AT}) \quad (3)$$

The corresponding unit concentration direct soil oral ingestion intake relation in PHAS3 is

$$\text{TAKE} = \text{SIR} \times \text{Afta} \times (1/\text{PERK}) \times (1-\exp[-\text{PERK}]) \quad (4)$$

TAKE = Unit concentration intake for this route, mg/day per mg/kg in soil  
 SIR = oral ingestion of soil from site in kg/day  
 Afta = adjustment factor for scenario conditions, dimensionless  
 PERK = ED x LP, where ED is the time duration of exposure to pollutant at the residence, and LP is a first-order decay constant. PERK is dimensionless; LP has units of time<sup>-1</sup>.

The major differences between equation (2) and (4) are twofold; the location of variables and the terms with PERK. In equation (4),  $(1/\text{PERK}) \times (1-\exp[\text{PERK}])$  accounts for the environmental process that deplete pollutant concentration in soil over a period of time. The RAGS equation does not include this term; pollutant decay in environmental media is assumed to be minimal in the exposure period. In mathematical terms, as PERK approaches zero,  $(1/\text{PERK}) \times (1-\exp[\text{PERK}])$  approaches one.

In PHAS3, the unit concentration intake is computed for each route. These intakes for a scenario are summed to determine an overall intake for the chemical, here called SUMTAKE. The applicable public health criterion now enters the assessment. The product (PHLD x BW) is a daily intake limit of that chemical. This limit divided by SUMTAKE is a concentration term called the preliminary pollutant limit value (PPLV):

$$\text{PPLV} = \text{PHLD} \times \text{BW} / \text{SUMTAKE} \quad (5)$$

SUMTAKE and the PPLV are related to the hazard index. From the above discussion, RAGSTAKE and TAKE are related:

$$\text{RAGSTAKE} = \text{CS} \times \text{TAKE} / \text{BW} \quad (6)$$

as are their summations

$$\text{Sum(RAGSTAKE)} = \text{CS} \times \text{SUMTAKE} / \text{BW} \quad (7)$$

Both sides can be divided by PHLD, with these equivalent results:

$$\begin{aligned} \text{Hazard Index} &= \text{Sum(RAGSTAKE)} / \text{PHLD} = \text{CS} / \text{PPLV} \\ &= \text{SUMTAKE} \times \text{CS} / (\text{PHLD} \times \text{BW}) \end{aligned} \quad (8)$$

From equation (8), the PPLV is the concentration corresponding to a hazard index of unity. PHAS3 uses the last relation in equation (8) to provide a hazard index per unit concentration for assessment purposes.

In 1990, the companion document to RAGS, the Human Health Evaluation Manual, Volume I, Part B<sup>3</sup>, was issued to address risk-based preliminary remediation goals. The conceptual approach is the same as of that in RAGS, except that the objective is reversed. In RAGS, the hazard index was sought for a known concentration. In Part B, a concentration is computed that will meet the criterion that the hazard index = 1. For water or sediment remediation, equation (8) shows that the PPLV is that concentration. For soil remediation, the problem is somewhat more complicated, and is discussed below.

## 2.2 PHAS3 Treatment of Special Situations.

The treatment in Section 2.1 has been general in scope. In this section, situations which require adjustment to this treatment are discussed.

### 2.2.1 Hazardous Land Sites

PHAS3 handles three different source media of contamination: water, sediment, and soil. A hazardous land site is the most complex, in that it can pose a multidimensional problem in respect to contamination location and receptor. For example, subsurface soil contamination can be a source for pollutant intake via groundwater as a potable water source while surface and near-surface soil contamination can be a source for pollutant intake via direct soil exposure. The concentrations can differ markedly from one soil stratum to another. PHAS3 assigns soil strata or locations to pathways as indicated in Table 1. PHAS3 is more comprehensive than is RAGS, which does not address the issue of different soil sources at a waste site. The utility of a single PPLV for soil renovation guidance would be suspect if several soil strata were involved in a scenario. Thus, a PPLV is computed for each stratum (see Section 2.3.2 for interpretation differences).

### 2.2.2 Dermal and Respired Pollutant Intake

Strictly, equation (8) is specific for one mode of human exposure. PHAS3 is oriented to oral intakes, and as discussed below, other intake modes are adjusted to an oral basis. The PPLV can still be defined by equation (5), where the PHLD is understood to be based on oral intake.

TABLE 1. PHAS3 Exposure Pathways in Order of Presentation

<u>PATHWAYS</u>  (Routes shown in parentheses)	<u>Environmental Medium</u>		
	<u>Water</u>	<u>Topsoil</u>	<u>Sediment</u>
Domestic water use, surface water supply. (consumed water alone or combined with either or both inhaled vapor intake and dermal absorption)	Yes	Yes <sup>a</sup>	Yes
Water recreation (ingested water alone or combined with either or both inhaled vapor intake and dermal absorption)	Yes	Yes <sup>b</sup>	Yes
Fish consumption	Yes	Yes <sup>b</sup>	Yes <sup>d</sup>
Vegetable consumption	Yes	Yes <sup>b</sup>	
Beef consumption (water alone or with plant intake included) <sup>c</sup> (plant alone or with either or both soil and water) <sup>c</sup>	Yes ---	--- Yes <sup>b</sup>	
Milk consumption (water alone or with plant intake included) <sup>c</sup> (plant alone or with either or both soil and water) <sup>c</sup>	Yes <sup>d</sup> ---	--- Yes <sup>b</sup>	
Dust intake in vicinity of on-site residence		Yes <sup>a</sup>	
Dust intake at an on-site work setting		Yes <sup>e</sup>	
Inhaled pollutant in house from vapors diffused from soil		Yes <sup>f</sup>	
Inhaled pollutant at on-site location from vapors diffused from soil		Yes <sup>g</sup>	
Inhaled pollutant at off-site location from vapors diffused from soil		Yes <sup>g</sup>	
Domestic water use, groundwater supply. (consumed water alone or combined with either or both inhaled vapor intake and dermal absorption)		Yes <sup>g</sup>	

- a. Soil at site causing pollution designated as #1 subsite topsoil.  
b. Soil at site causing pollution designated by user. Options  
are #1 subsite topsoil or #2 subsite topsoil.  
c. Reference is to exposure routes to the steer or cow.  
d. No further exposure pathways for this medium.  
e. Soil at site causing pollution designated as #2 subsite topsoil.  
f. Soil at site causing pollution designated as basement subsoil portion.  
g. Soil at site causing pollution designated as diffusion/infiltration  
subsoil portion.



Following RAGS, the hazard index is the sum of component hazard indices, each of which deals with sums of RAGSTAKE by mode of exposure. Each hazard index is  $\text{Sum}[(\text{RAGSTAKE})_{\text{mode}} / \text{PHLD}_{\text{mode}}]$ .  $\text{PHLD}_{\text{mode}}$  is expressed in consistent terms for each mode (see page 8-5 in RAGS). An equivalent approach is to introduce  $\text{PHLD}_0$  into each non-oral hazard index term. For the specific example of the inhalation mode, subscripted "i", the result is:

$$\text{Hazard Index} = (\text{PHLD}_0 / \text{PHLD}_i) \times [\text{Sum}(\text{RAGSTAKE})_i / \text{PHLD}_0].$$

From the properties of summation, the term  $\text{PHLD}_0/\text{PHLD}_i$  can adjust all inhalation RAGSTAKE terms, and from equation (6), all inhalation TAKE terms. With this term included, equation (8) still applies. In PHAS3 equations (see Appendix B), the term  $\text{PHLD}_0/\text{PHLD}_i$  is called CFIO, and the analogous dermal term is called CFDO.

### 2.2.3 Time-Related Terms

Pollutants can be transformed and thus removed as specific entities from an environment source by processes such as photolysis, chemical or microbial reactions. Moreover, the pollutant transfer rate from a medium to another by diffusion is concentration dependent. As concentration decreases with time, so will the projected intake of a pollutant by end-point human receptors. For example, equation (4) indicates that TAKE for the ingestion of soil with chemical is a time-dependent function, since the value of PERK is defined in part by the exposure time ED. The time intake basis for valuation of PPLV or a hazard index in PHAS3 must be precisely stated.

In Figure 1, the curve  $\text{TAKE}_j(t)$  represents the unit concentration intake for a route or path "j". A time-averaged intake,  $\text{TAKE}_j(\text{avt})$ , is defined as:

$$\text{TAKE}_j(\text{avt}) = (1/t) \int_0^t \text{TAKE}_j(t) dt \quad (9)$$

and is used in PHAS3 as the time-related intake. Note that equation (9) indicates that for a given exposure time interval, a specific time-averaged intake is computed. The point at which the time-averaged value  $\text{TAKE}_j(\text{avt})$  is positioned on the  $\text{TAKE}_j(t)$  curve between time zero and a specific time  $t_2$  is shown in Figure 1. Time  $t_x$  is the ordinate of that point. The curve  $\text{SUMTAKE}(t)$  is also shown in Figure 1. The value  $\text{SUMTAKE}(\text{avt}_2)$  occurs on the  $\text{SUMTAKE}(t)$  curve at time  $t_{\text{sum}}$ . The  $\text{SUMTAKE}(\text{avt}_2)$  value would be used in equation (8) to compute a hazard index or a PPLV.

$\text{SUMTAKE}(\text{avt})$  should be computed as the sum of component scenario  $\text{TAKE}_j(t)$ , with subsequent integration of equation (9). The operation can be difficult, if not impossible, to do in closed form. The PHAS3 approach assumes that the order of summation and integration are interchangeable:  $\text{SUMTAKE}(\text{avt})$  is computed as the sum of individual  $\text{TAKE}_j(\text{avt})$  values. If this assumption was correct, in Figure 1,  $t_x$  and  $t_{\text{sum}}$  would coincide with each other.

Another consequence of time-averaged intake is that prior to the time  $t_{\text{sum}}$ , actual daily intake exceeds the time-averaged intake. Assessors should check that intake in this early portion of the exposure period is not so excessive

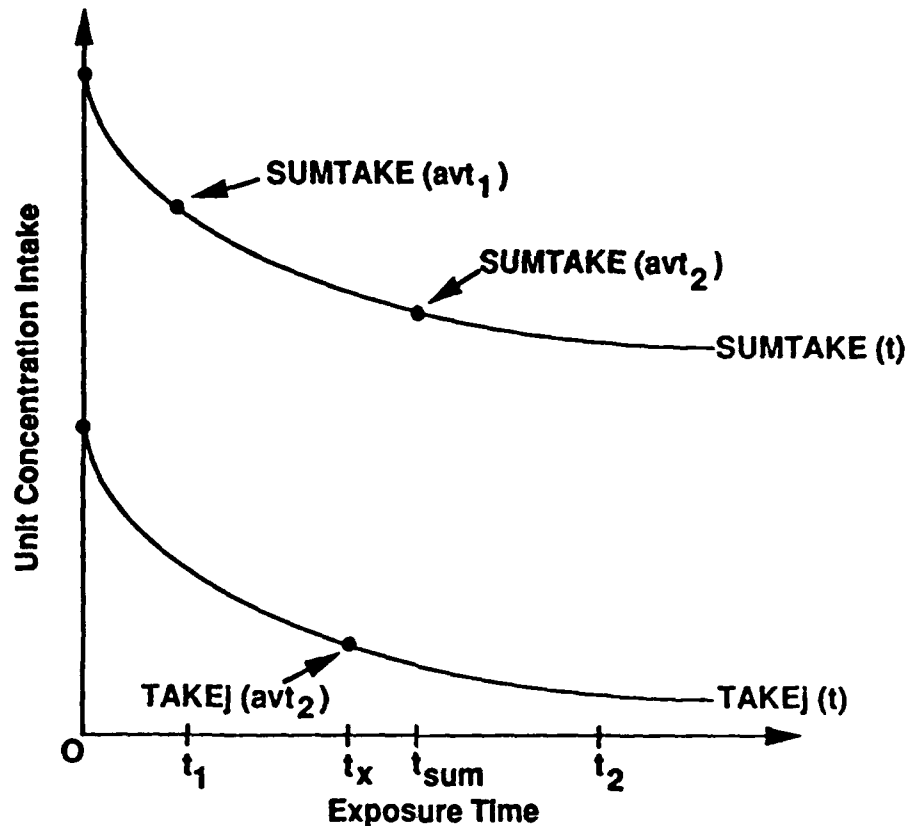


Figure 1. Unit Intake Curves Illustrating the Impact of Time Dependency.

as to be of public health concern. This can be done in PHAS3 by substituting a shorter exposure time frame, such as  $t_1$ , and computing  $SUMTAKE(av_1)$ .

A related concern is short-term exposure to children vs. long-term exposure to adults. For a given scenario, the intake by children is less than that of adults. But as a rule, the intake is more than would be expected from a body weight to body weight comparison. The limiting intake for a child is the product  $PHLD \times BW$ , where both factors are based on the child. The child  $PHLD$  is often the same as for an adult, but  $BW$  is clearly less. The author recommends that, where applicable, that both a child-based and adult-based analysis be performed. PHAS3 is devised so that both analyses can be easily done in one pass-through.

## 2.3 PHAS3 Applications

### 2.3.1. Remedial Investigation Planning and Performance

The term "preliminary" in PPLV also applies to PHAS3. It should be most useful at the start of a remedial investigation exercise. It can resolve questions of analysis sensitivity; clearly problems can occur in assessment credibility if a proposed analytical method cannot detect a substance at the PPLV concentration. The PPLV can serve a detection goal for selection of analytical methodology.

In the scenario formulation process, PHAS3 provides a "blueprint" to indicate the data inputs for the exposure assessment. The blueprint indicates data that are employed in unit concentration intake equations, as well as data that may be used for estimation purposes. Thus, while every identified datum may not be necessary for the investigation, the planner is aware of the data requirements for different estimation options. The constraint analyses provide "red flags" that the user may want to address in depth as part of the environmental evaluation in the remedial investigation.

As data are developed in the remedial investigation, files can be created with PHAS3 for their storage. Documentation concerning the source of data can be concurrently stored. PHAS3 may be used directly for a formal remedial investigation exposure assessment with three caveats: first, the exposure pathways are included in the PHAS3 repertoire (Table 1); second, the assumptions involved in PHAS3 exposure pathway equation development apply to the specific site situation; and third, that approval is obtained from the appropriate regulatory authority.

### 2.3.2 Visualization of Public Health Data

The comparison of PPLV and CS can be extended to more than one chemical substance. For water or sediment media or simpler land site problems, the comparison is easy to visualize. Figure 2 shows an example for a site with two contaminants; the concentration of each contaminant can be thought of as a dimension in a mathematical space. The PPLVs (points A and B) are located on the axes. If the contaminants have additive effects (an assumption made in the absence of knowledge to the contrary), a line between the PPLVs defines the unit hazard index, a boundary between what is "clean" and what may not be "clean". Survey results expressed as representative concentrations can be viewed as points in the two-dimensional concentration space. If a point is "inside" the boundary, such as point C in Figure 2, the hazard index corresponding to point C is less than 1.

For a situation with more than two substances, visualization becomes difficult. However, the mathematics still are straightforward. If the PPLVs for compounds 1, 2, ..., n are PPLV1, PPLV2, ..., PPLVn, the CS1, CS2, ..., CSn sets that meet the hazard index = 1 criterion satisfy the equation

$$(1/\text{PPLV1}) \times \text{CS1} + (1/\text{PPLV2}) \times \text{CS2} + \dots + (1/\text{PPLVn}) \times \text{CSn} = 1 \quad (10)$$

Survey representative concentrations for the compounds can be inserted to determine if the specific sum exceeds or is less than one.

For more complex land site problems, this comparison for all compounds can't be done in one step. Rather, an analogous process is done for each compound. In Figure 2, in place of substances, there are soil strata, and in place of a PPLV for each substance, there is a PPLV for each soil stratum. With those differences, the steps described above can be done on a substance by substance basis to compute each substance's hazard index, but the summation to compute the hazard index for all substances must be performed as a separate step.

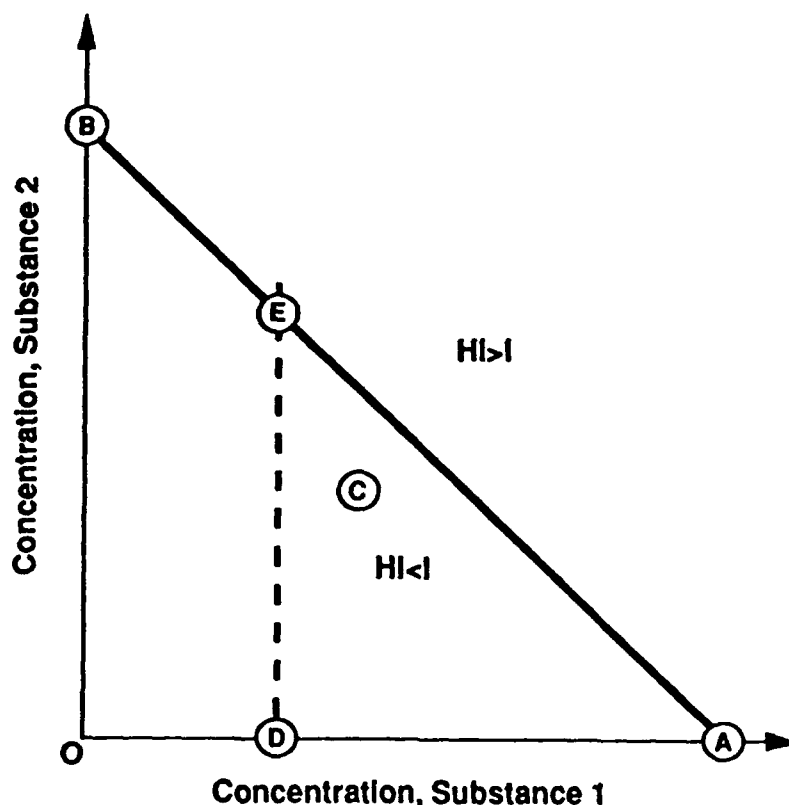


Figure 2. Relation of the PPLVs of Two Pollutants to Hazard Index and Type 1 Constraints.

### 2.3.3 Integration of Non-Public Health Effects

PHAS3 provides the user with an elementary analysis of biota data to indicate adverse effects within a hazard index-defined space. Since the criteria for such effects are typically in concentration units (such as mg/L in water causing a certain threshold toxicity to fish within a lifetime), they are more readily contrasted to a PPLV than to a dose or hazard index. Figure 2 shows a simple example of this contrast. The criterion for an adverse effect of "substance 1" at concentration = D appears as the vertical line D-E. If there was only an adverse effect of "substance 2", the concentration involved would be shown as a horizontal line. In PHAS3 terminology, if line D-E intersects the triangular area O-A-B, a type 1 constraint situation could exist; potentially, the biota criterion may dictate the extent to which remediation is necessary. This situation is shown in Figure 2, where the pollutant concentrations define the point C as discussed in Section 2.3.2. But point C is outside the area O-B-E-D, an area in which two conditions are met: (1) hazard index < 1 and (2) the concentration of "substance 1" < D.

More complex cases could be advanced, such as adverse toxic effects on fish for both substances. If the substances' toxicities were additive, a line connecting the values on each axis could be constructed. Then, the Type 1 constraint condition could occur if the triangular area O-A-B were intersected by the toxicity line.

### 3.0 DESCRIPTION OF PHAS3 STRUCTURE

#### 3.1 Hardware

PHAS3 operates on a computer system with 640 K capacity controlled by MS-DOS at level 3.1 or higher. It requires a BASIC interpreter program such as GW-BASIC (with which it was developed), IBM BASICA, or a more contemporary version. PHAS3 is designed to operate with several different storage device configurations (see Section 4.1). A printer with 8.5-inch wide paper is required, and, as a minimum, an 80-column wide monochrome monitor. PHAS3 software is normally supplied on either a high-density 5.25 inch floppy disk or a 3.5 inch diskette.

#### 3.2 Definitions

To avoid ambiguities, some terms are specifically defined. These are:

data - numerical values stored in external files.

dataname - Title used in PHAS3 to describe a given datum.

DOS - MS-DOS used to manage computer operations.

download - As a verb, the act of transferring data or information from an external file for processing in PHAS3 programs. Also used as an adjective (downloaded) to indicate information or data so transferred and online.

external file - a collection of information or data created and stored for use in PHAS3 programs. Each file has a specific file name and extension.

information - numerical values or text used for purposes other than as inputs to PHAS3 intake equations or estimation methods.

medium - a repository of a pollutant in the environment that is subject to remediation. Thus, the user may process pathways involving exposure via water when soil is the definitive medium.

online - capable of being transferred within PHAS3 programs (programmers call this attribute COMMON or GLOBAL).

#### 3.3 System Structure and External Files

PHAS3 programs are designed to process external files that contain scenario information, non-chemical data, and chemical-related data. These files can be created at one time and recalled for use. Three specific types of files are used and are differentiated by their filename extension. The extensions will be used in the text for description, and are:

.PXX	.PXX files store two numeric information lists. The first keeps track of pathways involved in a given scenario. This list is called the Scenario Selection Table (SST). The second list describes the role of data in route exposure or constraint calculations. It is called the Data Use Status Table (DUST).
------	---

There are three varieties of this file based on medium: .PWA for water assessments, .PTS for soil assessments, and .PSD for sediment assessments. A text information line can be used to identify and provide commentary about the scenario developed.

**.LDS** .LDS files contain 175 numeric entries, the non-chemical data in an exposure assessment analysis. The data include human and livestock consumption factors, site soil parameters, watershed descriptors, non-chemical model parameters for transfers between soil, water, and air, and air dispersion model results. Along with each numeric entry, the user can include information to document the source or derivation of data. A commentary text line is provided to identify the site.

**.DAT** .DAT files contain 75 numeric entries, the chemical-related data. The data include PHLD values, input physicochemical data for estimation methods, partition coefficients, soil to air or water transfer model output data as well as first-order decay constants, and biota limit data inputs to constraint test equations. Along with each numeric entry, the user can include information to document the source or derivation of data. A commentary text information line is provided to identify the pollutant and provide other needed information.

PHAS3 programs can create, download, and store files as well as change file contents. The ERASE or DELETE utilities in DOS, or the KILL command within the GW-BASIC interpreter, can be used to remove files.

Figure 3 is a schematic of PHAS3 structure. Entry to and exit from PHAS3 is via OPEN3. Access between any of the "planet programs" is through OPEN3. Additionally, CRDES3 can be accessed from OPEN3 to do chemical-related data estimations in a "desk calculator" mode; in this mode, estimations are not retained online. This access is shown by the solid-line one-way arrow. Section 4.3 details OPEN3 operations.

In PATWAY3, scenarios for the exposure assessment process are defined. For this purpose, exposure route information is extracted from a satellite PTXXX3 program\* based on the route repertoire for a specified medium. Scenario information can be stored in a .PXX file. A .PXX file can be used in the two data-handling programs NOCH3 and CHMF3 as a "filter", whereby only data required for assessments, or data from which such required data can be estimated, are handled. This is shown by the dashed-line one-way arrow directed from a .PXX file to these programs; information downloaded from a .PXX file in either NOCH3 or CHMF3 is not retained when these programs are exited. A .PXX file can be either downloaded or created in PATWAY3 for online use. Online information can be passed to OPEN3 as shown by the solid-line single-arrow in Figure 3. PATWAY3 accesses satellite programs to provide a "blueprint" of data needs for a selected scenario: PTLL3 to provide a hardcopy

\* PTXXX3 represents the generic name of one of three programs: PTWAT3, which addresses water medium exposure pathways, PTTOP3, for soil medium exposure pathways, and PTSED3, for sediment medium exposure pathways.

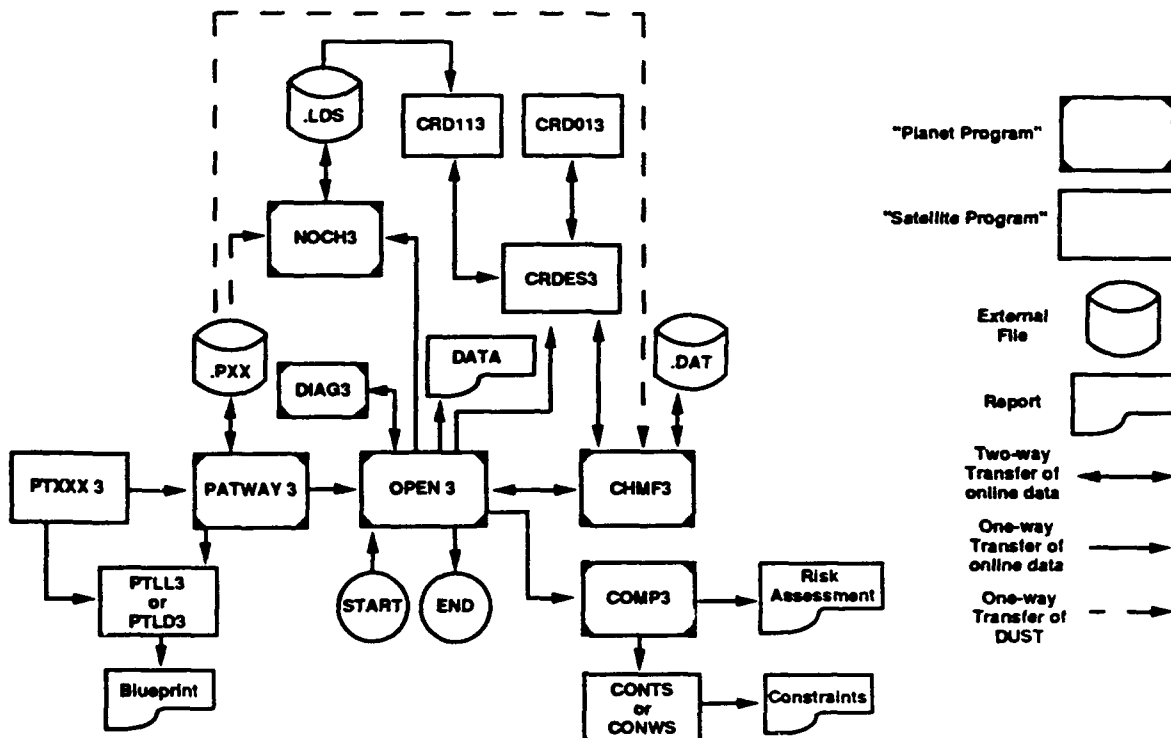


Figure 3. PHAS3 System Structure and Program-File Relationships

"blueprint" or PTL3 to write the "blueprint" as a user-designated external file (see Section 5.5 for details). The blueprint describes the data significance, and shows how data can be obtained, either from external sources or from routines in NOCH3 or accessed from CRDES3. Section 5 details PATWAY3 and its satellite programs operations.

The two data-processing programs are NOCH3 and CHMF3. Their operations are detailed in Sections 6 and 7, respectively. NOCH3 downloads data from .LDS files, alters data online, and store online data in a user-specified .LDS file. CHMF3 does similar operations with .DAT files. In addition, CHMF3 can access CRDES3 for data estimates via its satellite programs, and these estimates are retained online.

Section 8 describes the program DIAG3, which lets the user (1) review on monitor the information sets from a downloaded .PXX file or data sets from downloaded .LDS and .DAT files; (2) obtain hardcopy reports of data used in analyses and documentation; (3) review online datanames and values and (4) change dataname values and documentation.

COMP3 contains the unit concentration intake equations and computes assessment parameters. COMP3 accesses the satellite program CONWS to optionally analyze either or both of the two contingencies described in Section 2 for water or sediment. COMP3 accesses the satellite program CONTS to do similar analyses for soil. Section 9 describes COMP3, CONWS, and CONTS operations.

CRDES3 provides background information about chemical-related data and accesses estimation subroutines in the satellite programs CRD013 and CRD113. CRDES3 and CRD013 operations are detailed in Section 10, while CRD113 operations are detailed in Section 11. When CRDES3 is accessed from CHMF3; data estimated within CRDES3 can be retained online. When CRDES3 programs are accessed from OPEN3; estimates are not retained online after CRDES3 is exited. If chemical-related data are needed for estimation subroutines and CRDES3 is accessed from CHMF3, online data are employed. The user supplies chemical-related input data when CRDES3 is accessed from OPEN3. The subroutines in CRD113 require data from a .LDS file. CRD113 can download a .LDS file (see above), and the downloaded file data will be online after CRDES3 is exited. This feature is not indicated in Figure 3.

#### 4.0 PHAS3 INSTALLATION AND START UP

##### 4.1 Installing PHAS3

PHAS3 software is supplied in ASCII code on either a high-density 5-1/4 inch floppy disk or a 3-1/2 inch diskette. The supplied software is partitioned into the subdirectories \PHAS3\DISK1 and \PHAS3\DISK2. The files in \PHAS3\DISK1 include the programs shown in Table 2. The files required in subdirectory \PHAS3\DISK2 are DEFLPWA.PWA, NULFIL.PWA, DEFLPTS.PTS, DEFLPSD.PSD, DEFAULT.LDS, DEFCHEM.DAT, and PROMPT.OPE.

Most modern computer systems comprise of at least one installed hard disk drive and at least one removable disk or diskette drive. This minimal configuration is assumed in the following discussion. In theory, PHAS3 can be operated with both subdirectories on a disk or diskette, but this is not recommended. The user can create and add external files to the \PHAS3\DISK2 subdirectory, which can exceed the available disk or diskette storage limits.

The installation procedure is described below. Figure 4 indicates the DOS commands corresponding to this description.

1. Decide the device for \PHAS3\DISK1 subdirectory files (the disk 1 device). This can be a disk, diskette, or a subdirectory partition on a hard disk. If it is a disk or diskette, first format the device. If a hard disk is used, create the subdirectory partition (here, its name is assumed to be \PHAS3\DISK1). GWBASIC.EXE should be on the disk 1 device; if it is a hard disk, either in the \PHAS3\DISK1 subdirectory or accessible to it via a PATH statement. Copy all the files in the \PHAS3\DISK1 subdirectory on the supplied hardware to the disk 1 device.
2. Decide the device for \PHAS3\DISK2 subdirectory files (the disk 2 device). If it is a disk or diskette, format the device. On a hard disk, there are two options for designating the disk 2 device, either as a separate subdirectory partition or the disk 1 device subdirectory partition. If the first option is selected (which is recommended), create the subdirectory partition (here, its name is assumed to be \PHAS3\DISK2).
3. Copy the contents of \PHAS3\DISK2\ to the disk 2 device.



TABLE 2. FILES SUPPLIED ON SUBDIRECTORY \PHAS3\DISK1

.BAS Files				.SCN Files				.CMP Files Continued			
CHMF3	BAS	11616	4-01-93	BASEVAP	SCN	1334	2-08-93	HENRY	CMP	1265	11-10-92
COMP3A	BAS	15564	3-05-93	CONTSOIL	SCN	1332	2-08-93	KD1INFO	CMP	1538	11-12-92
CONTS	BAS	8425	4-02-93	DOMWAT	SCN	1334	2-08-93	KOCINFO	CMP	1212	11-23-92
CONWS	BAS	5437	3-03-93	FISH	SCN	917	2-08-93	KPATINFO	CMP	1327	11-12-92
CRD013	BAS	25365	3-08-93	GNDOMWAT	SCN	1293	2-08-93	KPDINFO	CMP	744	11-10-92
CRD113	BAS	17285	4-07-93	LIVESTOK	SCN	1406	9-29-92	KPMINFO	CMP	870	11-23-92
CRDES3	BAS	9583	4-07-93	MILK	SCN	1468	9-29-92	KSPKSV	CMP	1221	11-12-92
DIAG3B	BAS	9027	4-01-93	OPENWAT	SCN	1335	2-08-93	KWPVINFO	CMP	1137	11-12-92
INSTALL	BAS	1898	1-21-93	PATINFO	SCN	738	2-08-93	LEBASA	CMP	785	10-02-90
NOCH3	BAS	14246	3-26-93	PATPHP	SCN	6196	1-17-92	LOGKOW	CMP	1162	11-12-92
OPEN3	BAS	7941	3-19-93	RESSOIL	SCN	1134	11-16-92	LPDSS	CMP	1368	11-12-92
PATWAY3	BAS	7833	3-03-93	SITEVAP	SCN	1198	2-08-93	LPSED	CMP	1234	11-12-92
PTLD3	BAS	18041	4-07-93	TOFFSITE	SCN	1130	2-09-93	LPTS12	CMP	1331	11-12-92
PTLL3	BAS	16834	4-07-93	VEGGIE	SCN	880	2-08-93	LPWAT	CMP	1094	11-12-92
PTSED3	BAS	2955	3-04-93					MILLERM	CMP	1139	11-12-92
PTTOP3	BAS	11301	3-04-93					MILTBOIL	CMP	2112	3-31-93
PTMAT3	BAS	5143	3-04-93					MKDIFFA	CMP	1386	11-18-92
				.NCI Files							
				FILE1	NCI	10914	11-24-92	MKROINFO	CMP	1528	12-15-92
				FILE2	NCI	7648	11-24-92	MKSW5	CMP	1209	11-13-92
				FILE3	NCI	5628	11-24-92	MKSW6	CMP	1441	11-18-92
				FILE4	NCI	7372	10-23-92	NOLWT	CMP	1382	11-13-92
				FILE5	NCI	6018	10-26-92	ORGLEP	CMP	1357	11-13-92
				FILE6	NCI	8798	10-30-92	PERMINFO	CMP	892	11-13-92
				FILE7	NCI	9764	11-24-92	PHYTOTOX	CMP	1176	11-13-92
				FILE8	NCI	9294	11-02-92	STATDEX	CMP	225	12-15-92
				FILE9	NCI	5853	11-24-92	STOREIT	CMP	594	10-26-92
				FILEX	NCI	2670	3-25-92	TAFINFO	CMP	868	11-13-92
								TBOIL	CMP	1142	11-10-92
								TMELT	CMP	575	11-10-92
								VAPMENU	CMP	1311	11-10-92
								VAPRINFO	CMP	1438	4-06-93
								VPFACTOR	CMP	204	7-21-88
								VPTABLE	CMP	1314	10-12-90
								WATERSOL	CMP	1231	11-13-92
				.OPE Files							
ASSIGN	OPE	5	12-07-92								
CHEMFILE	OPE	1252	3-31-93								
CHEMPROP	OPE	1315	2-10-93								
COMPUTE	OPE	1331	2-10-93								
DIAGNOST	OPE	1112	2-10-93								
NOCHFL	OPE	1431	2-10-93								
OVERVIEW	OPE	1528	2-10-93								
PARAM	OPE	11393	3-24-93								
PATHWAY	OPE	1454	2-10-93								
PROMPT	OPE	436	1-06-92								
								.CMP Files			
				AQUATOX	CMP	1197	11-09-92				
				BAFINFO	CMP	1046	12-08-92				
				BCFINFO	CMP	1113	11-23-92				
				CATLIST	CMP	1682	2-16-93				
				CATTOX	CMP	1327	11-10-92				
				CONTTALK	CMP	1254	11-02-92				
				DAINFO	CMP	934	4-06-93				
				DTDCINFO	CMP	1109	11-12-92				
				DTDSINFO	CMP	1366	11-18-92				
				DTICINFO	CMP	1425	11-18-92				
				DTISINFO	CMP	1462	11-12-92				
				DTOCINFO	CMP	1318	11-18-92				
				DTOSINFO	CMP	1443	11-10-92				
				DWINFO	CMP	776	3-31-93				
				EXPSEQ	CMP	1136	11-17-92				
				FOCINFO	CMP	1052	11-23-92				
				.BAT Files							
PHAS	BAT	15	1-14-92								

ASSUME: Drive A: PHAS3 SOFTWARE LOADING DISKETTE DRIVE (5.25" OR 3.5")  
Drive C: PHAS3 SOFTWARE STORAGE HARD DRIVE

(User entries are in bold letters)  
C>PROMPT \$P\$G  
C:\>**MKDIR C:\PHAS3**  
C:\>**CHDIR C:\PHAS3**  
C:\PHAS3>**MKDIR DISK1**  
C:\PHAS3>**CHDIR DISK1**  
C:\PHAS3\DISK1>**COPY A:\PHAS3\DISK1\\*.\***  
C:\PHAS3\DISK1>**CHDIR C:\PHAS3**  
C:\PHAS3>**MKDIR DISK2**  
C:\PHAS3>**CHDIR DISK2**  
C:\PHAS3\DISK2>**COPY A:\PHAS3\DISK2\\*.\***  
C:\PHAS3\DISK2>**CHDIR C:\PHAS3\DISK1**  
C:\PHAS3\DISK1>**GW BASIC INSTALL**  
4 (response to installation menu prompt)  
c:\phas3\disk2\ (response to prompt to identify subdirectory)

Figure 4. Command Sequence to Install PHAS3 as Described in Section 4.1

4. Define the current directory to the disk 1 device. Then, at the DOS prompt, type 'gwbasic install'. The program INSTALL starts, and the following menu is displayed:

\*\*\*\*\* INSTALLATION MENU \*\*\*\*\*

This program assigns a disk drive or subdirectory for external data files (Disk 2 Device). Once assigned, that drive or subdirectory will be accessed by the system.  
Enter an option from 1 to 4....

Input '1' for A: drive  
Input '2' for B: drive  
Input '3' to put all files on this subdirectory  
Input '4' to put .PXX, .LDS, and .DAT files on a different subdirectory.  
Enter your selection:

If the response is '1', '2' or '3', no further inputs are required, and the user is returned to DOS. If option '4' is selected, the program prompts for the full subdirectory name in which the contents of Disk 2 will reside. For example, if the hard disk is the "C" drive, the entry would be c:\phas3\disk2\ . A final backslash is required. After the subdirectory name entry, the user is returned to DOS.

#### 4.2 System Notes and Programming Conventions

PHAS3 has been designed with user-friendly features. It provides online messages describing program subsections, and explains and prompts for user inputs. Operational user inputs are either integer numeric entries, alphanumeric entries, or filenames. After a user input, the return (enter) key is depressed. Halts are provided to permit the user to review, and at the

user's option, to print the contents of a screen display (Shift-PrintScreen). After such halts, the return key is depressed to continue processing; this keystroke is called a continuation return.

User inputs are monitored to detect common errors. PHAS3 informs the user when such an error occurs. Common errors which are detected include:

- \* An integer is entered that is outside the range of accepted values.
- \* A non-integer is entered when an integer is specified.
- \* An unspecified alphanumeric entry (typographical error) is entered.
- \* A filename is entered that violates DOS specifications.
- \* A filename to be downloaded is not accessible.

In the case of the first four errors above, PHAS3 will continue processing after the error is resolved. Moreover, if an alphanumeric entry is entered when a numeric entry is expected, or vice versa, the interpreter issues the message "?Redo from start". When this happens the disputed input should be checked, the error determined, and the correct input re-entered (followed by a return). The last error listed above may lead to exit from PHAS3, particularly when the file involved is supplied software. Appendix C discusses such errors and their probable resolution.

Specific conventions are followed in the narrative. Program names, file extensions, and specific filenames are shown in capital letters.

PHAS3-generated messages or prompts are shown in compressed font

(compressed font) Such messages and prompts appear in quotes when used within text narrative. User responses to PHAS3 prompts are shown in single quotes; in practice, they are entered without quotation marks, and are followed by pressing the return (enter) key. Alphanumeric responses are shown in lower case; the user can respond in either case. If a term is in braces "<term>", the specific contents of the displayed term will be determined by PHAS3. The text "term" explains or paraphrases the braced display.

#### 4.3 OPEN3

If the disk 1 device is a removable disk or diskette, ensure that the device is in the correct drive. If the disk 1 device is a hard disk, assign execution to the \PHAS3\DISK1 partition. If the disk 2 device is a removable disk or diskette, ensure that the device is in the correct drive. At the DOS prompt, enter 'phas'. The monitor first displays "basic open3", and after a short pause, the "OPEN3 Main Selection Menu" shown in Figure 5 appears.

The menu accepts a prompt value between 1 and 10 (except 6 and 8) to start a specific function. Entries '2', '3', '4', '5', '7', and '9' respectively access programs PATWAY3, NOCH3, CHMP3, DIAG3, COMP3, and CRDES3.

```

***** POLLUTANT HAZARD ASSESSMENT SYSTEM (PHAS) *****
          Version 3, October 1992
***** OPEN3 MAIN SELECTION MENU *****

```

```

ENTER      FUNCTION PERFORMED BY ENTRY
1      Descriptions of PHAS and its component programs.
2      SCENARIO definition and PATHWAY selections.
3      NON-CHEMICAL data processing.
4      CHEMICAL-RELATED data processing.
5      Diagnostic utility. Review scenarios, review
      or alter online data, or printout data.
7      EXPOSURE ASSESSMENT and optional constraint analysis.
9      Chemical data estimation methods, results not online.
10     Exit the system to DOS.
ENTER YOUR SELECTION::

```

Figure 5. OPEN3 Main Selection Menu

If entry '1' is selected, the display shown below appears:

```

***** PROGRAM EXPLANATION MENU *****
ENTER      EXPLANATION
0      None, exit to Main Function Selection Menu
1      Overall system description
2      Scenario and pathway processing (PATWAY3)
3      Non-chemical data processing (NOCH3)
4      Chemical-related data processing (CHMF3)
5      Hazard Assessment and Constraint Analyses (COMP3)
6      The DIAGNOSTIC UTILITY routines (DIAG3)
7      Chemical-related data estimation methods (CRDES3)
ENTER YOUR SELECTION::

```

Enter the number for the desired explanation message. At the conclusion of a message, enter a continuation return to return to this menu.

PHAS3 is exited by responding with '10' to the OPEN3 Main Selection Menu prompt. The prompt must be confirmed by responding 'yes' to the query "Are you leaving PHAS? ". A 'no' response directs the user to the OPEN3 Main Selection Menu. A 'yes' response directs the user to DOS.

## 5.0 PATWAY3

PATWAY3 is accessed when '2' is entered at the OPEN3 Main Selection Menu prompt. The initial display is shown in Figure 6. The status report indicates the last downloaded file, last stored file, last file operation, and current medium selection. The initial display in Figure 6 indicates that no file has been either downloaded or stored. The selection menu accesses six functions in PATWAY3, and the option to exit to OPEN3. With the exception of selection '0', after the completion of any function operation, either the entire format in Figure 6 or the PATWAY3 Main Selection Menu is displayed.

### 5.1 Source Medium Selection

PATWAY3 initial default is the "surface or near surface soil" medium. For a different medium, select function '1'. The following message will appear:

```
***** SOURCE MEDIUM SELECTION *****
PHAS3 computes intake per unit concentration and a preliminary pollutant
limit value (PPLV) for pathways involving surface water, groundwater, or
sediment as the source of the pollutant. In the case of soil, more than
one PPLV may be computed, depending on the extent of soil contamination
(different sites, subsoil vs. topsoil contamination). Select the source
medium for pollutant from the 3 options below (integer input).
INTEGER      MEDIUM
    1      Surface water or groundwater
    2      Surface or near-surface soil
    3      Sediment (as a contamination source for surface water only).
Enter your selection here::
```

Enter the integer for the desired medium. The PATWAY3 Main Selection Menu will then appear. The medium is then indicated by the ".PXX" entry at the menu's option line: "6 Store SST/DUST in a <.pxx> - extension file"

### 5.2 Stored Filenames Review

Select '2' at the PATWAY3 Main Selection Menu prompt to list existing files on the Disk 2 device with the current .PXX extension.

---

```
***** WELCOME TO PATWAY3, THE SCENARIO OPERATIONS MODULE *****
***** FILE STATUS REPORT *****
Last downloaded file was ** .pts
Last stored file was ** .pts
Last file manipulation **
Current medium selection is ** Surface and near-surface soil pathways
***** PATWAY3 MAIN SELECTION MENU *****
ENTER      FUNCTION PERFORMED BY ENTRY
    1      Select a different environmental medium
    2      Review files with current extension
    3      Download file with current extension
    4      Create a scenario SST and DUST
    5      Produce scenario report (on disk or hard copy)
    6      Store SST/DUST in a .pts-extension file
    0      Exit to OPEN3 Now
Enter function number::
```

Figure 6. Initial Display of the PATWAY3 Main Selection Menu

### 5.3 Stored File Downloading

If selection '3' to the "PATWAY3 Main Selection Menu" is chosen, the list of files described above is displayed, and is followed by this query:

Enter pathway input file (w/o .pxx extension)::

With correct input, the file is downloaded, and this message is displayed:

```
Scenario information downloaded from file <filename.pxx>
***** PATHWAYS IN FILE <disk or subdirectory:filename.pxx>
Scenario Title: <alphanumeric>
Medium is <medium>
```

Execution pauses for a continuation return, after which a short narrative of pathways involved in the downloaded scenario appears. After another continuation return, the routine ends.

PATWAY3 attempts to resolve improper filename inputs. If the file name specified is not on the disk 2 device, an explanation message is issued, the current list of files is displayed, and the file name input prompt again appears. If the file name entered has illegal characters (for example, punctuation within a file name), the same procedure occurs.

### 5.4 Scenario Creation

Select function '4' to create files. The following lines are displayed:

```
***** SCENARIO CONSTRUCTION ROUTINE *****
Enter Scenario Title Line::
```

The user can enter scenario title information that can occupy up to 255 alphanumeric spaces maximum; this sized entry would occupy the rest of the prompt line plus 2-1/2 additional lines. As the user completes a line on the display, the display "wraps-around" to the next line. The cursor back, cursor forward, backspace, insert and delete keys suffice for most editing purposes. The return key terminates input regardless of cursor position.\*

After the title line entry, the user is guided through a series of exposure pathway selection displays. Each display explains the pathway and prompts for an entry. The pathway is omitted from consideration by the '0' entry. Based on the pathway options, the pathway can be included (with no options, this is always the '1' entry) or, with multiple exposure route options, one option is selected (the input will range from '1' to as high as '4'). Table 1 summarizes the pathways and routes in order of appearance.

At the conclusion a successful scenario creation, the user is returned to the File Status Report, and the message displayed at the line "Last file manipulation." reads "New SST/DUST online only." If the user has, either by error or deliberately, omitted all pathways, the message "WARNING! Null scenario(no paths)!" is displayed, and the user is returned to the main selection menu.

\* The size of text entry and the editing specifications also apply to title lines and documentation messages entered in NOCH3 and CHMF3.

### Surface and Near Surface Soil Subsite Selections

A hazardous waste site may cover a sizable area in which the soil type may differ, or it may contain more than one drainage watershed, where exposure routes could involve different watersheds (homes could be located in one watershed and crop fields in another). PHAS3 allows the user to "split-up" the topsoil layer at a site into two subsite parcels. In Table 1, the pathways with footnote "b" are allocated by subsite. For such pathways, the pathway selection prompt discussed above is followed by a second prompt:

Which subsite is involved, #1 or #2? Enter '1' or '2':

The domestic water, surface source pathway is assigned to subsite #1. Other pathway subsite selections must conform with this assignment. If this pathway is not included in the scenario, subsites can be assigned in any consistent order. If the meat (beef) pathway is included in a scenario, its subsite designation is used for the milk consumption pathway; when the prompt sequence for the milk consumption pathway occurs, the subsite option is not displayed. If the meat pathway is not selected, but the milk pathway is, the prompt sequence for the milk pathway includes the subsite option prompt.

### 5.5 The Scenario Data Needs Report

After function '5' is selected at the "PATWAY3 Main Selection Menu" prompt, PATWAY3 checks the status of the online SST and DUST. If a valid DUST is not online, this message appears:

No pathways selected, can't printout/write. Try another option.

and the PATWAY3 Main Selection Menu is presented. Otherwise, the following message and selection menu is presented:

```
PATHWAY INFORMATION FOR SCENARIO <user input information> IN MEDIUM <medium>
SCENARIO NEEDS REPORT OUTPUT OPTIONS SELECTIONS
Enter '1' for lineprinter output.
Enter '2' for 'Disk 2 device file' output. Enter selection::
```

If you enter '1' to the prompt, a message to check the printer is issued:

Make sure that your line-printer is operating!  
Hit enter (return) to continue...

The program PTL3 is entered, and execution proceeds without user inputs.

If option '2' is selected, PTL3 is accessed. This message appears:

```
Welcome to the disk-drive file output program PTL3.
You will create an ASCII file for review with any word processor
You will be prompted to enter a filename on the 'Disk 2' device
This filename will be used to store the report on disk.
NOTE -- File size for stored report can be large (up to 70K).
Review device ** <Disk 2 device> ** for space availability, and manage files.
Program will list existing stored report files now
```

If stored report files exist (extension .STO), they are listed. If none exists, this message appears: "There are no .STO files currently in storage"

After either response, the prompt "Enter filename for storage (w/o extension)::" appears, to which the user provides a filename without the extension. After a valid filename, PTLD3 operates without further user input.

Both PTL3 and PTLD3 provide identical monitor responses. These are discussed as part of the sample problem below. At the conclusion of either program, the File Status Report and PATWAY3 Main Selection Menu appears for the next function selection.

To illustrate PHAS3 operations, this sample problem is processed. It is also employed in subsequent illustrations of displays and printouts.

" There is an area of a former ammunition plant where soil is contaminated with 'trinitroanything', a persistent organic compound, at concentrations up to 2 mg/kg. A decision is needed as to whether this concentration is 'safe' for current land use; if not, remediation may be necessary. The area consists of farm residences and grazing areas for cattle, raised primarily for beef. The portion of the area used for cattle grazing drains to a creek, from which water is diverted to feed the animals. There is concern about vapor exposure due to diffusion of trinitroanything from soil to the living area in homes, and about exposure to dust in and about homes. The residents raise some of their vegetables in gardens near their homes."

Surface and near surface soil is the source medium. Thus, at the PATWAY3 Main Selection Menu prompt, no change of source medium is required. The scenario creation routine (Section 5.4) is entered by responding with '4' to the menu. The following pathways (see Table 1 for order of appearance) are selected :

- \* Vegetable consumption. Gardens are selected to be at the #1 subsite.
- \* Meat consumption. There are 3 options, and the option to include all routes is chosen. The specific area for grazing is assumed to be in the #2 subsite.
- \* Dust intake in the vicinity of on-site residence
- \* Inhaled vapors in house from vapors diffused from soil

Portions of the printed "Pathway Selection And Data Needs Summary" report are in Figure 7. After the scenario title and medium are listed, "global data" are identified. These data are used to determine the limiting intake from which the PPLV and hazard index are computed (equation 5 in Section 2.3). After the "global data" list, each exposure pathway is identified. After each pathway identification, datanames are listed in two groups. The first list appears after the title line

"DATA USED IN INTAKE EQUATIONS ARE..."

These listed data are explicit inputs to the corresponding intake equation in Appendix B (see "Caution" message below). Each dataname line is preceded by an index integer. This index is required in the DIAG3 program if the user wants to manually change data (see Section 8.5). Table 3 shows the index and datanames assigned in PHAS3.



# SCENARIO DATA NEEDS REPORT

For the 'Sample problem for manual discussion' scenario in Surface and near-surface soil pathways

## \*\*\*\*\* SPECIAL ABBREVIATIONS \*\*\*\*\*

dwb = dry weight basis

nodim = dimensionless

p.c. = partition coefficient

## GLOBAL DATA INVOLVED IN ALL PATHWAYS INTAKES ARE...

- 1 BWa, adult body weight, kg
- 26 BWc, child body weight, kg
- 176 DTol, Long-term limit dose estimate, oral basis, mg/kg-day
- 177 DTos, Short-term limit dose estimate, oral basis, mg/kg-day
- 185 TAF, Long term averaging time adjustment code  
(pathways 8, 9, and 11 data needs omitted)

PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.  
Exposure assumed to be primarily caused by inhalation of vapors in basement.

## DATA USED IN INTAKE EQUATIONS ARE...

- 18 BIRa, adult inhalation rate, basement vapors, m<sup>3</sup>/day
- 43 BIRC, child inhalation rate, basement vapors, m<sup>3</sup>/day
- 63 AFlt, Time adjustment factor, long-term (adult), topsoil paths
- 64 AFst, Time adjustment factor, short-term (child), topsoil paths
- 77 Teta, Time exposure for adult, topsoil pathways, days
- 148 Ab3, basement area contacting soil diffusing vapors, m<sup>2</sup>
- 171 MXb, dilution air factor for vapor flux in basement, day/m<sup>3</sup>
- 178 DTil, Long-term limit dose estimate, inhalation basis, mg/kg-day
- 179 DTis, Short-term limit dose estimate, inhalation basis, mg/kg-day
- 233 MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m<sup>2</sup>-day
- 234 MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m<sup>2</sup>-day

\*\*\*\*\*

## DATA WHICH CAN BE USED TO ESTIMATE EQTN. DATA ARE...

- 78 Tetc, Time exposure for child, topsoil pathways, days
- 141 foc3, fraction organic carbon, soil contiguous with basement
- 142 rh3, bulk density, soil contiguous with basement, kg/L
- 143 th3, soil fraction voids with water, basement model, L/L
- 144 ep3, soil fraction voids with air, basement model, L/L
- 145 db, initial top of pollution layer below grade, basement model, m
- 146 hb, lower depth of pollution layer, basement model, m
- 147 Qa3, volume air through basement, m<sup>3</sup>/day
- 186 MW, Molecular weight, g/mol
- 187 Tm, Normal or extrapolated melting point, deg C
- 188 LogP, Log (base10) octanol-water partition coefficient
- 189 Wsol, Water solubility, mg/L
- 190 Tb, Normal or extrapolated boiling point, deg C
- 191 VP, Saturated vapor pressure, mm Hg
- 192 Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)
- 206 Da, Molecular diffusivity in air, m<sup>2</sup>/sec
- 208 Kh, Henry Law constant, dimensionless [conc./conc.]
- 217 Kd3 soil/water p.c. for basement subsoil, mg/kg / mg/L
- 225 LPds, persistence rate constant for diffusion-layer subsoils, 1/year

Figure 7. Sections from Sample Problem "Pathway Selection and Data Needs Summary Report. (page 1 of 3 pages)

DATA USED IN CONSTRAINT EQUATIONS ARE...

88 Uwm, water intake by steer, L/day  
 89 Upm, plant (forage) intake by steer, kg (dwb)/day  
 90 Usm, soil intake by steer, kg/day  
 91 Uwd, water intake by dairy cow, L/day  
 92 Upd, plant (forage) intake by dairy cow, kg (dwb)/day  
 93 Usd, soil intake by dairy cow, kg/day  
 94 BWM, representative steer body weight, kg  
 95 BWD, representative dairy cow body weight, kg  
 112 rh1, bulk density, topsoil #1 subsite, kg/L  
 113 th1, average moisture capacity, topsoil #1 subsite, L/L  
 127 rh2, bulk density, topsoil #2 subsite  
 128 th2, average moisture capacity, topsoil #2 subsite, L/L  
 211 Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L  
 212 Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L  
 215 Kd1 soil/water p.c. for #1 subsite pathways, mg/kg / mg/L  
 216 Kd2 soil/water p.c. for #2 subsite pathways, mg/kg / mg/L  
 232 MKro2, model soil/water p.c., #2 subsite runoff, mg/kg / mg/L  
 241 TOL, Organoleptic limit - taste in water, mg/L  
 243 AQTL, Aquatic toxicity limit in water, mg/L  
 244 PHLW, Phytotoxicity limit in water, mg/L  
 245 PHLS, Phytotoxicity limit in soil, mg/kg  
 246 focPS, foc for soil used to determine phytotoxicity limit  
 247 CTael, Cattle toxicity adverse effects limit, mg/kg-day

\*\*\*\*\*

1 Bwa, adult body weight, kg

The DEFAULT.LDS value for Bwa is 70 kg (about 154 pounds), a frequently used weight based on the averaged weight of the adult man and woman across an age spectrum from 18 years to 75 years. Based on EFH89, EPA 600/8-89/043, a more precise value is 71.8 kg (not adjusted for population within age group). This reference may be consulted for more specific sex or age group data.

10 Wva, adult vegetable consumption, kg dwb/day

Wva is the vegetable consumption for adults from produce grown at a contaminated site (or with contaminated water). It is cited on a dry-weight basis. The report PPLVM, TR8918, DTIC AD-A206976 describes approaches to developing an estimate as does EFH, EPA/600/8-89/043. See RAGS1-SUPP91, OSWER 9285.6-03, PB91-921314, for Superfund Guidance. The value 0.017 kg/day in DEFAULT.LDS represents intake by adults in rural, non-farm areas of vegetables (including potatoes). Estimates for other generic locales are in Table 13 of the above citation. Consult EFH, EPA/600/8-89/043 for fruit intake data.

11 Wma, adult beef consumption, kg/day

Wma is the adult daily consumption of beef from animals raised at a contaminated site. A value of 0.044 kg/day is in DEFAULT.LDS, from the presentation in the EFH, EPA 600/8-89/043. This is developed primarily for farm households. Further guidance about obtaining estimates for particular locales is in that handbook. For Superfund Guidance, consult RAGS1-SUPP91, OSWER 9285.6-03, PB91-921314.

Figure 7. Sections from Sample Problem "Pathway Selection and Data Needs Summary Report. (page 2 of 3 pages)

176 DTol, Long term limit dose estimate, oral basis, mg/kg-day

DTol is a chronic oral limit dose used in PHAS for adult public health assessments. It is a 'global' variable and also adjusts inhalation and dermal intakes to an oral basis. DTol conceptually equals the reference dose (RfD) used by EPA in Chapter 7, RAGS1-IF89 (EPA/540/1-89-002). DTol represents (1) the daily dose at which no toxic effect occurs within a lifetime OR, (2) for known or suspect carcinogens, a safe-sided dose for a finite acceptable risk level (ARL) of cancer incidence within a 70-year lifetime. The ARL should be stated in documentation.

Usually, DTol is based on toxicity or bioassay studies with mammals. For toxic effects, No-Effect Adverse Dose Level (NOAEL) is defined. The NOAEL is divided by uncertainty factors to estimate DTol. RAGS1-IF89 provides guidance as to how these factors are assigned. For a carcinogenic-based DTol, tumor incidence-dose data is required. A math model is often employed to process data (the common output is a 'q\*' value where  $DTol = ARL/q^*$ ). These procedures are beyond the scope of PHAS programs.

The EPA maintains the Integrated Risk Information System (IRIS) as an online computer service to provide data for substances that have been studied and the study results interpreted.

233 MKdba, soil flux p.c., basement model long-term, mg/kg per  $mg/m^2$ -day

MKdb and MKdo are 'super' soil-air p.c. for diffusion of pollutant from a contaminated soil column to bulk air. They indicate the mg/kg in soil which generates a time-averaged flux of  $1 mg/m^2$ -day. This flux is multiplied by an area ( the area normal to the flux ) to yield a mg/day time averaged source term.

MKdb is used in the intake equation for the inhalation of vapors diffused from soil indoors (basement) pathway. MKdo is used in two intake equations dealing with the inhalation of vapors diffusing from soil while outdoors either onsite or offsite. The same algorithm is used to compute MKdb and MKdo. The non-chemical input data to evaluate them in CRD113 are: th, rh, and ep (subscript 3 for basement, 4 for other pathways), hb (or ho), db (or do), and exposure time T<sub>ETA</sub> or T<sub>ETC</sub>. Kd3 (for basement) or Kd4 (for other pathways) Kh, Da, and LPdss are chemical-data inputs. The CRD113 method uses landfarming equations cited in SEAM88 (EPA/540/1-88/001), pages 20-21. The underlying diffusion model is discussed in the User's Manual, Section 11.5.

NOTE: \*1\* If CRDES3 was accessed from OPEN3, the user provides chemical-related data. \*2\* All non-chemical data are accessed from a .LDS file. \*3\* LPdss is involved in the computation of MKdb or MKdo, which are time-averaged terms.

.....  
\*\*\*\*\* SUBSITE OPTION SELECTIONS \*\*\*\*\*  
Subsite #1 Vegetable Intake Pathway.  
Subsite #2 Beef Intake Pathway.

Figure 7. Sections from Sample Problem Pathway Selection and Data Needs Summary Report. (page 3 of 3 pages)

Table 3. Datanames and Symbols Used in PHAS3. (page 1 of 4 pages)

Index	Identification of Dataname
1	BWa, adult body weight, kg
2	IWa, adult drinking water intake, L/day
3	EIWa, adult oral water equiv. for inhaled pollutants, L/day
4	DAWa, adult body surface for dermal exposure to water, m <sup>2</sup>
5	DETa, adult dermal exposure time to domestic water, hr/day
6	OIWa, swimwater ingested by adult, L/TA day
7	ORWa, adult inhalation rate during water activity, m <sup>3</sup> /TA day
8	ODTa, adult water activity immersion time, hour/TA day
9	Wfa, adult fish consumption, kg/day
10	Wva, adult vegetable consumption, kg dwb/day
11	Wma, adult beef consumption, kg/day
12	Wda, adult milk consumption, L/day
13	SIRa, adult oral intake of soil, residential, kg/day
14	SARa, adult exposure area to dust on skin, residential, m <sup>2</sup>
15	PLa, adult perspiration rate, L/m <sup>2</sup> /day
16	OIRa, adult inhalation rate, onsite residential, m <sup>3</sup> /day
17	CSI, construction area-related dust intake, kg/workday
18	BIRa, adult inhalation rate, basement vapors, m <sup>3</sup> /day
19	EIRa, adult inhalation rate, offsite residential, m <sup>3</sup> /day
26	BWc, child body weight, kg
27	IWc, child drinking water intake, L/day
28	EIWc, child water oral water equiv. for inhaled pollutant, L/day
29	DAWc, child body surface for dermal exposure to water, m <sup>2</sup>
30	DETC, child dermal exposure time to domestic water, hr/day
31	OIWc, swimwater ingested by child, L/TA day
32	ORWc, child inhalation rate for water activity, m <sup>3</sup> /TA day
33	ODTC, child water activity immersion time, hr/TA day
34	Wfc, child fish consumption, kg/day
35	Wvc, child vegetable consumption, kg/day
36	Wmc, child beef consumption, kg/day
37	Wdc, child dairy consumption, L/day
38	SIRc, child oral intake of soil, residential, kg/day
39	SARc, child exposure area to dust on skin, residential, m <sup>2</sup>
40	PLc, child perspiration rate, L/m <sup>2</sup> /day
41	OIRc, child inhalation rate, onsite residential, m <sup>3</sup> /day
43	BIRc, child inhalation rate, basement vapors, m <sup>3</sup> /day
44	EIRc, child inhalation rate, offsite residential, m <sup>3</sup> /day
51	SLA, soil loading rate on exposed skin, kg/m <sup>2</sup> /day
52	RSPA, particulate conc in air, residential, kg/m <sup>3</sup>
53	CWTF, weather/time factor for construction site soil pathway
54	WECF, wind erosion climatic factor, unitless
55	PEF, soil particulate inhalation efficiency factor
61	AFwa, Time adjustment factor, long-term (adult), water paths
62	AFwc, Time adjustment factor, short-term (child), water paths
63	Afta, Time adjustment factor, long-term (adult), topsoil paths
64	Aftc, Time adjustment factor, short-term (child), topsoil paths
65	AFsa, Time adjustment factor, long-term (adult), sediment paths
66	AFsc, Time adjustment factor, short-term (child), sediment paths

Table 3. Datanames and Symbols Used in PHAS3. (page 2 of 4 pages)

Index	Identification of Dataname
74	TEca, Time exposure for adults, construction pathway, days
75	TEwa, Time exposure for adults, water pathways, days
76	TEwc, Time exposure for child, water pathways, days
77	TEta, Time exposure for adult, topsoil pathways, days
78	TEtc, Time exposure for child, topsoil pathways, days
79	TEsa, Time exposure for adults, sediment pathways, days
80	TEsc, Time exposure for child, sediment pathways, days
86	fm, fat content in beef
87	fd, fat content in milk
88	Uwm, water intake by steer, L/day
89	Upm, plant (forage) intake by steer, kg (dwb)/day
90	Usm, soil intake by steer, kg/day
91	Uwd, water intake by dairy cow, L/day
92	Upd, plant (forage) intake by dairy cow, kg (dwb)/day
93	Usd, soil intake by dairy cow, kg/day
94	BWM, representative steer body weight, kg
95	BWD, representative dairy cow body weight, kg
101	foc5, fraction organic carbon content of sediment
102	rh5, bulk density of sediment, kg/L
103	th5, void fraction of sediment, L/L
104	dp5, initial top of pollution layer in sediment below grade, m
105	hp5, bottom depth of pollution layer in sediment below grade, m
106	As5, surface area of contaminated sediment in waterway, ha
107	Qu5, annual flow of waterway below polluted sediment locale, m <sup>3</sup> /sec
111	foc1, fraction organic carbon, topsoil #1 subsite
112	rh1, bulk density, topsoil #1 subsite, kg/L
113	th1, average moisture capacity, topsoil #1 subsite, L/L
114	Acw1, contaminated area of #1 subsite, ha
115	Aw1, total watershed area at #1 subsite outfall, ha
116	WP1, wilt point, topsoil #1 subsite
117	FC1, field capacity, topsoil #1 subsite
118	K1, erodability factor for #1 subsite
119	LS1, length-slope factor for #1 subsite
120	C1, crop cover factor for #1 subsite
121	P1, erosion control factor for #1 subsite
122	RO1, runoff from #1 subsite, inches/year
123	Qu1, Annual ave. flow above #1 subsite outfall, m <sup>3</sup> /sec
124	R1, rain/runoff factor for contaminated site
126	foc2, fraction organic carbon, topsoil #2 subsite
127	rh2, bulk density, topsoil #2 subsite
128	th2, average moisture capacity, topsoil #2 subsite, L/L
129	Acw2, cont. area for watershed #2 site, ha
130	Aw2, total watershed area at #2 subsite outfall, ha
131	WP2, wilt point, topsoil #2 subsite
132	FC2, field capacity, topsoil #2 subsite
133	K2, erodability factor for #2 subsite
134	LS2, length-slope factor for #2 subsite
135	C2, crop cover factor for #2 subsite
136	P2, erosion control factor for #2 subsite

Table 3. Datanames and Symbols Used in PHAS3. (page 3 of 4 pages)

Index	Identification of Dataname
137	RO2, runoff from #2 subsite, inches/year
138	Qu2, Annual ave. flow above #2 subsite outfall, m <sup>3</sup> /sec
141	foc3, soil fraction organic carbon, basement model
142	rh3, soil bulk density, basement model, kg/L
143	th3, soil fraction voids with water, basement model, L/L
144	ep3, soil fraction voids with air, basement model, L/L
145	db, initial top of pollution layer below grade, basement model, m
146	hb, lower depth of pollution layer, basement model, m
147	Qa3, volume air through basement, m <sup>3</sup> /day
148	Ab3, basement area contacting soil diffusing vapors, m <sup>2</sup>
151	UW3, wind-speed for on-site exposure to diffusing vapors, m/sec
152	foc4, soil fraction organic carbon, outside diffusion
153	rh4, soil bulk density, outside diffusion, kg/L
154	th4, soil fraction voids with water, outside diffusion, L/L
155	ep4, soil fraction voids with air, outside diffusion, L/L
156	do, initial top of pollution layer below grade, outside diffusion, m
157	ho, lower depth of pollution layer, outside diffusion, m
158	AO4, area of site for outside diffusion/infiltration, ha
159	UW4, wind-speed for off-site exposure to diffusing vapors, m/sec
160	MH, rep. mixing height, on-site, m
161	DW4, distance from site to off-site receptors, m
162	MH4, rep. mixing height for off-site receptor, m
163	TK6, pollutant thickness in soil column (groundwater infiltration), m
164	RI6, infiltration of rainwater to aquifer, m/year
165	VGW6, velocity of groundwater flow, m/year
166	TAQ6, thickness of aquifer, m
167	th6, effective porosity in aquifer, L/L
171	MXb, dilution air factor for vapor flux in basement, day/m <sup>3</sup>
172	MXon, dilution air factor for vapor flux to outside on-site, day/m <sup>3</sup>
173	MXof, dilution air factor for vapor flux off-site, day/m <sup>3</sup>
174	MXef, windblown particle rate to offsite receptors, kg/m <sup>2</sup> -day
176	DTol, Long-term limit dose estimate, oral basis, mg/kg-day
177	DTos, Short-term limit dose estimate, oral basis, mg/kg-day
178	DTil, Long-term limit dose estimate, inhalation basis, mg/kg-day
179	DTis, Short-term limit dose estimate, inhalation basis, mg/kg-day
180	DTdl, Long-term limit dose estimate, dermal basis, mg/kg-day
181	DTds, Short-term limit dose estimate, dermal basis, mg/kg-day
185	TAF, Long-term averaging time adjustment code
186	MW, Molecular weight, g/mol
187	Tm, Normal or extrapolated melting point, deg C
188	LogP, Log (base10) octanol-water partition coefficient
189	Wsol, Water solubility, mg/L
190	Tb, Normal or extrapolated boiling point, deg C
191	VP, Saturated vapor pressure, mm Hg
192	Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)
193	Kav, Soil/vegetable p.c., mg/kg (dwb) per mg/kg soil
194	Ksp, Soil/plant (forage) p.c., mg/kg (dwb) per mg/kg soil
195	foc for soil used to determine soil/veg p.c.
196	foc for soil used to determine soil/forage p.c.

Table 3. Datanames and Symbols Used in PHAS3. (page 4 of 4 pages)

Index	Identification of Dataname
197	Kpat, Plant(forage) to adipose tissue p.c.,mg/kg per mg/kg dwb
198	BCF, Fish Bioconcentration [in water] factor, mg/kg fish per mg/L
206	Da, Molecular diffusivity in air, m <sup>2</sup> /sec
207	Dw, Molecular diffusivity in water, m <sup>2</sup> /sec
208	Kh, Henry Law constant, dimensionless [conc./conc.]
209	PC, Dermal permeability constant, cm/hr
210	BAF, Fish bioaccumulation factor, mg/kg fish per mg/L
211	Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L
212	Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L
213	Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb)
214	Kpd, Plant (forage) to milk p.c., mg/L milk per mg/kg (dwb)
215	Kd1 soil/water p.c. for #1 subsite pathways, mg/kg / mg/L
216	Kd2 soil/water p.c. for #2 subsite pathways, mg/kg / mg/L
217	Kd3 soil/water p.c. for basement subsoil, mg/kg / mg/L
218	Kd4 soil/water p.c. for outside diffusion, mg/kg / mg/L
219	Kd5 sediment/water p.c., mg/kg / mg/L
221	LPwat, persistence rate constant for surface water, 1/year
222	LPsed, persistence rate constant for sediment, 1/year
223	LPts1, persistence rate constant for #1 subsite soil, 1/year
224	LPts2, persistence rate constant for #2 subsite soil, 1/year
225	LPdss, persistence rate constant for diffusion-layer subsoils, 1/year
231	MKro1, model soil/water p.c., #1 subsite runoff, mg/kg / mg/L
232	MKro2, model soil/water p.c., #2 subsite runoff, mg/kg / mg/L
233	MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m <sup>2</sup> -day
234	MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m <sup>2</sup> -day
235	MKdoa, soil flux p.c., outdoors long-term, mg/kg per mg/m <sup>2</sup> -day
236	MKdoc, soil flux p.c., outdoors short-term, mg/kg per mg/m <sup>2</sup> -day
237	MKdwa, sediment/openwater p.c. long-term, mg/kg per mg/m <sup>2</sup> -day
238	MKdwc, sediment/openwater p.c. short-term, mg/kg per mg/m <sup>2</sup> -day
239	MKgwa, topsoil/groundwater p.c. long-term, mg/kg per mg/L
240	MKgwc, topsoil/groundwater p.c. short-term, mg/kg per mg/L
241	TOL, Organoleptic limit - taste in water, mg/L
243	AQTL, Aquatic toxicity limit in water, mg/L
244	PHLW, Phytotoxicity limit in water, mg/L
245	PHLS, Phytotoxicity limit in soil, mg/kg
246	focPS, foc for soil used to determine phytotoxicity limit
247	CTAEL, Cattle toxicity adverse effects limit. mg/kg-day

The second list of datanames appears after the

DATA WHICH CAN BE USED TO ESTIMATE EQTN. DATA ARE...

title line. These data may be needed in CRDES3 or NOCH3 routines to provide estimates for one or more of the route intake equation data. After each exposure pathway is processed, the following message appears on the monitor:

End listing for pathway: <description message for pathway>

After the pathway listings are completed, the next heading is

DATA USED IN CONSTRAINT EQUATIONS ARE...

The user will need these data to solve all type 1 constraints. Some of the datanames identified in the "Data used in Intake Equations" listings may also appear in this listing.

An information message is then printed for all identified datanames. The messages follow the sequence of the numerical index. The index from 1-175 is for non-chemical data. Each message printed indicates the significance of data, its value in DEFAULT.LDS, the basis for this value, and information on how it can be evaluated. The index from 175-250 is for chemical-related data. For these, each message printed out indicates the significance of the data, and what, if any, estimation methods are available in CRDES3. Otherwise, information is presented on how data can be obtained. At the conclusion of the information messages for non-chemical data, the following message appears on the monitor: "End of information messages for non-chemical data".

At the conclusion of the information message for chemical-related data, the message appears on the monitor: "End of information messages for chemical-related data"

If the medium is "surface or near-surface soil", the report will conclude with a listing headed "SUBSITE OPTION SELECTIONS" for subsite 1 and subsite 2 options the user selected.

CAUTION: If a dataname could be cited in both the "Data used in Intake Equation" list and the "Data which can be used to estimate eqtn. data" list, it will be omitted from the second list. The reader should not conclude that datanames on the "Data which can be used to estimate eqtn. data" list are inherently less important than those on the "Data used in Intake Equation" list. An important case is shown in the listings for Pathway 13 in Figure 7. The terms for exposure time (TEtc) and extent of contamination below grade (hb and db), are clearly important, but appear only on the second list. These terms don't explicitly appear in the Pathway 13 intake equation of Appendix B. Rather, they are used in the PHAS method for determining MKdba and MKdbc.

## 5.6 Scenario Information Storage

When function '6' is selected at the PATWAY3 Main Selection Menu prompt, the existing filenames are first displayed. Next, the user is prompted:

Enter an allowable name up to 8 alphanums w/o .pxx extension.  
Please don't use the name - defl<pxx>

In response to this prompt, a filename is entered. As with all MS-DOS filenames, it cannot exceed 8 characters in length (extension excluded). After a file is stored, one of two messages will appear. If the stored scenario is recently-created, the message is:



New SST/DUST stored on Disk 2 device file.  
Otherwise, the message is  
Online SST/DUST stored on Disk 2 device file.

CAUTION: DEFLPWA.PWA, DEFLPTS.PTS and DEFLPSD.PSD are protected. If one of them is entered at the above prompt, this message is displayed:

WARNING!! <default file for .pxx> is a read-only file. Choose another filename.  
and the user is prompted to enter an alternate filename.

## 6.0 NOCH3

NOCH3 is accessed when '3' is entered to the OPEN3 Main Selection Menu prompt. The NOCH3 initial display is shown in Figure 8. The status report is updated as NOCH3 operations are executed. The NOCH3 selection menu presents five functional routines, and the option to exit directly to OPEN3. The user enters the integer for the desired routine.

### 6.1 Download a .LDS File and Return to OPEN3 ("Load and Go")

Function '1' allows the user to download a specified .LDS file and return to OPEN3. This option is useful when an assessment is to be performed with an established non-chemical data base, or if the user prefers to modify data in DIAG3 (see Section 8.5) rather than in NOCH3. The names of available files are shown, and filename input (without the .LDS extension) is prompted. After the file is downloaded, the OPEN3 Main Selection Menu appears. This operation will be noted in the display: "Your last file operation was \*\* Downloaded 'to go' file." This line can be viewed in DIAG3 (Section 8.3), the next time NOCH3 is entered, in COMP3 (Section 9.0), or in CRD113 (Section 11.0).

---

```
***** WELCOME TO THE NON-CHEMICAL DATA PROCESSING PROGRAM (NOCH3) *****
***** FILE STATUS REPORT *****
Last downloaded file was **
Title of current online file (if any) is **
Last stored file was **
Last file operation was **
***** NOCH3 MAIN SELECTION MENU *****
ENTER  FUNCTION PERFORMED
  1    Download a stored .LDS file, immediate return to OPEN3
  2    Modify online information under DUST control.
  3    Modify a stored .LDS file under DUST control.
  4    Create a file for online use or storage
  5    Go to Storage options routine
  0    Exit NOCH3 with return to OPEN3
Enter selection:: 3
***** CURRENT INVENTORY OF .LDS FILES AT DEVICE...\phas3\disk2\
D:\PHAS3\DISK1
DEFAULT .LDS      DOWNLOAD.LDS      DDTFILE .LDS
6498304 Bytes free

Enter file name (w/o .LDS extension):: ddtfile
Downloading of file \phas3\disk2\ddtfile.lds completed...
*** NOCH3 DATA USE STATUS TABLE (DUST) LOAD MENU ***
You need a DUST to process data. Select one of these options.
Option '1' to use the online scenario DUST.
Option '2' to use the DUST from a stored file.
        The program prompts you for a file name.
Option '3' to use default DUST for selected environmental medium
Enter the desired option integer::
```

Figure 8. NOCH3 Main Selection Menu Display

## 6.2 .LDS File Retrieval, Data Review and Change Procedures

NOCH3 creates, modifies and stores non-chemical data files. NOCH3 data processing is performed under "DUST control". Not every datum is required for a given scenario, and one DUST control function is to omit those definitely not required. Some non-chemical data enter directly into input equations while other data are to estimate values of non-chemical or chemical-related data used in such equations. Another DUST control function is to indicate the role of data in a given analysis. The DUST for "DUST control" comes from either a .PXX file or online scenario information (that was either previously downloaded or developed in a current PHAS session).

All data review and changes performed in NOCH3 start with a downloaded .LDS file. The major differences between functions '2', '3', or '4' are when and from where a .LDS file is retrieved for review or change. The steps common to these functions are: 1. obtain the online data from a .LDS file, 2. obtain a DUST, and 3. do data review and changes.

### Obtain the online data from a .LDS file

Function 2: Data are online if an .LDS file has been previously downloaded in program NOCH3 or CRD113 (see Section 3.3) in a current session of PHAS3. NOCH3 checks for the presence of online data. If such data are available, the procedure to obtain a DUST follows. If such data are not available, the message: "No valid online info, select another option" is issued, and the NOCH3 Main Selection Menu is displayed again.

Function 3: The current listing of .LDS files is displayed. The prompt: "Enter file name (w/o .LDS extension):" then appears. The user enters the filename to be downloaded. The display sequence for this function appears in Figure 8.

Function 4: The user first answers this prompt:  
This routine will wipeout online .LDS file data. OK(yes/no)::  
With a 'yes' response, the file DEFAULT.LDS is automatically downloaded. With a 'no' response, the NOCH3 Selection Menu is displayed again.

### Obtain a DUST

The following menu is displayed:

```
***** DATA USE STATUS TABLE (DUST) LOADING PROCESS MENU *****
You will need a DUST to process data. Select 1 of 3 options.
Option '1' to use the online scenario DUST
Option '2' to use the DUST from a stored file.
        The program will prompt you for a file name
Option '3' to use default DUST for selected environmental medium
Enter the desired option integer::
```

If there is an online scenario DUST, it was either created or downloaded in PATWAY3 in a current session of PHAS3. Following selection of option '1' to the DUST Loading Process Menu, this message appears:

Your online DUST is for medium ...<medium description>  
and scenario titled...<alphanumeric supplied by user>  
OK to continue? (yes or no)::

If the user responds 'yes', the "data review and change routine" described in the next subsection starts. If the user responds 'no', the DUST Loading Process Menu is again displayed.

If the user selects either option '2' or '3' from the DUST Loading Process Menu, the Source Medium Selection display shown in Section 5.1 appears. The instructions given there apply. After medium selection, this message appears:

YOU HAVE SELECTED MEDIUM <medium description>  
OK to continue? (yes or no)::

If the user responds 'no', the process is repeated. If option '2' is selected, a listing of files with the extension <.pxx> is displayed next. The user is prompted: "Input name of DUST file:."  
The user provides the filename without the .PXX extension.

If option '3' is selected, a "default" .PXX file is automatically downloaded (one of the protected files mentioned in Section 5.6). The downloaded DUST includes all pathways available for exposure from a medium (if the medium is "surface or near-surface soil", both subsites are used). Then, the "data review and change routine" described in the next subsection commences.

**CAUTION:** A user can select a different DUST and a different source medium from an online DUST and an online source medium. The DUST downloaded in NOCH3 is not retained for use in other programs when NOCH3 is exited. The medium selected in NOCH3 is not retained for use in other programs when NOCH3 is exited. The online DUST and source medium selection (whichever is applicable) remains online when NOCH3 is exited.

#### Data Review and Change Routine

The following instructions apply to datanames indexed from 1 to 170. See Section 6.4 for special instructions for datanames MXb, MXon, MXof, and MXef.

After the header display in Figure 9, the line:

" The last file processing action was \*\* <message>" appears. The message summarizes the last file processing done with an .LDS file, either in NOCH3 or in CRD113. The first prompt in this routine is:

The current title line for the downloaded file is <user-supplied title>  
Should this line be changed (y/n or no)?::

If the response is 'yes', the prompt: " Enter revised title line:." is issued. An informative title of up to 255 spaces (an example is shown in Figure 9) can be entered. Refer to Section 5.4 for editing details.

\*\*\*\*\* DATA REVIEW AND CHANGE ROUTINE \*\*\*\*\*

The last file processing action was: File downloaded for review/change mode  
The current title line for the downloaded file is:  
Default file for starting new .LDS file. Check user's guide for parameter value derivation.  
Should this line be changed (yes or no)?:: yes  
Enter revised title line:: THE TITLE LINE is provided for a summary description of the site for which data are presented in the .LDS file. This message occupies 255 alphanumeric spaces, the 'string' capacity in BASIC. GWBASIC will cut your message off if it exceeds this capacity.

.....  
1 BWA, adult body weight, kg = 70  
Documentation: BWA, default file, see file1.nci for basis of data.  
Main input variable to intake pathway eqtn.  
Select '1' to accept current value and documentation message.  
Select '2' to replace value  
Select '3' to change documentation message  
Select '4' to get info message about variable. Input selection:: 2  
Enter revised value:: ? 55.5

.....  
1 BWA, adult body weight, kg = 55.5  
Documentation: BWA, default file, see file1.nci for basis of data.  
Main input variable to intake pathway eqtn.  
Select '1' to accept current value and documentation message.  
Select '2' to replace value  
Select '3' to change documentation message  
Select '4' to get info message about variable. Input selection:: 1

.....  
2 IWA, adult drinking water intake, L/day = 1.6  
Documentation: IWA, default file, see file1.nci for basis of data.  
Main input variable to intake pathway eqtn.  
Select '1' to accept current value and documentation message.  
Select '2' to replace value  
Select '3' to change documentation message  
Select '4' to get info message about variable. Input selection:: 3  
Enter revised documentation message:: This is where you would document the source or derivation of a specific dataname. Note the the info message shown below is associated with data in DEFAULT.LDS.

.....  
2 IWA, adult drinking water intake, L/day = 1.6  
Documentation:  
This is where you would document the source or derivation of a specific dataname. Note the the info message shown below is associated with data in DEFAULT.LDS.  
Main input variable to intake pathway eqtn.  
Select '1' to accept current value and documentation message.  
Select '2' to replace value  
Select '3' to change documentation message  
Select '4' to get info message about variable. Input selection:: 4

The DEFAULT.LDS value for IWA is 1.6 L/day, which is about the mean daily intake determined in several surveys discussed in Drinking Water and Health (Safe Drinking Water Committee, National Academy of Sciences, Washington, DC, 1977). EPA Regulations often use a 2 L/day intake, to account for roundoff and adverse-casing, as does Superfund guidance. Factors which could influence the selection of an IWA value are climate (people drink more in hot climates), and bottled beverage intake (water from an uncontaminated water source). For more information, see EPH89 (EPA 600/8-89/043) or RAGS1-SUPP91 (OSWER 9285.6-03, PB91-921314)

.....  
2 IWA, adult drinking water intake, L/day = 1.6  
Documentation:  
This is where you would document the source or derivation of a specific dataname. Note the the info message shown below is associated with data in DEFAULT.LDS.  
Main input variable to intake pathway eqtn.  
Select '1' to accept current value and documentation message.  
Select '2' to replace value  
Select '3' to change documentation message  
Select '4' to get info message about variable. Input selection:: 1

Figure 9. Sample Display, NOCH3 Data Review and Change Routine

A sample portion of the data review and change routine is shown in Figure 9. For each dataname displayed, the following information is supplied: 1. the current value, 2. user-supplied documentation of the value basis, and 3. a role message, indicating data use in the assessment analysis. A role message consists of one or more of the following statements:

Main input variable to intake pathway eqtn.  
Var. may be needed to estimate intake main input variable.  
Variable is used in constraint analysis equation.

The user can select four options: accept the current datum value ('1'), replace the value ('2'), change the documentation message ('3') or see the information message about the datum ('4').

Until option '1' is selected, any other option can be done. After option '1' is selected, processing advances to the next highest indexed dataname selected by DUST control. If option '2' (replace value) is chosen, the message: "Enter revised value::" is displayed, and the replacement value is entered. After option '3' is selected, the message "Enter revised documentation message::" appears, and the user can enter up to 255 spaces (3 lines of screen) of information. This is shown in Figure 9; see Section 5.4 for editing details. If the user chooses option '4', an information message is displayed. This message also appears in the Scenario Data Needs Report and documents data selection for DEFAULT.LDS. The information message should not be confused with an user-supplied documentation entry.

If the user wants just to change a title, a "short cut" can be employed. The file NULFIL.PWA, included on Disk 2, can be downloaded using function '3' procedures. After title modification, the NOCH3 Selection Menu will be displayed; no other datanames are presented for processing.

### 6.3 The Data Storage Routine

This function, accessed by selection '5', is announced by the display:

\*\*\*\*\* STORAGE DISPOSITION MENU \*\*\*\*\*

You have three options available.

Select '0' if you don't want to store data on Disk 2 device.

Select '1' if you want to store data in a file with the same filename as  
the downloaded file had. This is recommended for MODIFYING a file.

Select '2' to store data under a different filename than the downloaded  
file had. This is recommended for storing NEW files.

NOTE: Database will be in online storage until a different file with the  
specified extension (.LDS or .DAT) is subsequently downloaded.

Enter your storage option::

If '0' is entered, the File Status Report and the NOCH3 Selection Menu displays appear. The last line of the status report will read:

Your last file operation was \*\* Any changes to online data are not stored.

If '1' is entered, the downloaded filename automatically becomes the filename for storage. The online data and title are written to that file. The File

Status Report and NOCH3 Selection Menu then appear. The filename on the first two lines of the status report will be the same and the last line will read:

Your last file operation was \*\* Replacing last downloaded file with online mod.

If '2' is entered, the current list of .LDS files on the Disk 2 device are displayed. The user is prompted:

Enter an allowable filename up to 8 alphanums w/o .LDS extension::

The user supplies a filename (see Section 5.3 for filename error resolution). The online data and title are written to that file. In this case, the last line of the File Status Report will read:

Your last file operation was \*\* File stored with user-given name.

**CAUTION:** DEFAULT.LDS is a read-only file, and PHAS3 will stop an attempt to store online data to it. This could occur if DEFAULT.LDS is downloaded, data changed, and then option '1' is entered at the Storage Disposition Menu prompt. In this case, the message: "DEFAULT.LDS is a reserved filename. Select another." is issued, and the user is returned to the Storage Disposition Menu.

#### 6.4 Data Review and Change Routine for Air Dispersion Terms

Datanames MXb , MXon , MXof , and MXef are indexed respectively 171, 172, 173 and 174. They represent air dispersion model results, and the user can either input values directly from models other than those in PHAS3, or use NOCH3 estimation methods. MXon and MXof are estimated by variants of box or dispersion model equations. The models in PHAS3 are, by necessity of software size, elementary, and the reader should review the assumptions associated with their use in the following subsections. MXon and MXof are equivalent in meaning to the ratio  $\% / Q$  in Turner's notation<sup>4</sup>.

Figure 10 shows a sequence of processing for MXon as an example of the routine. The first three options appear as previously described. The options continue:

Select '4' to get info message about variable

Select '5' to access estimation method routine. Input selection::

After the '5' response to the above input selection prompt, the user selects the estimation routine. At the completion of the routine, the routine's estimation replaces the previous value online, and the replacement is noted on the line: "<index number, dataname> = <estimate>"

##### 6.4.1 MXb

Only one estimation method is in PHAS3,  $MXb = .1/Qa^3$ . This method is based on the assumption that basement air is rapidly mixed with diffusing vaporized pollutant, and there are no "hot spots" where concentrations can build up.

##### 6.4.2 MXon

PHAS3 has two MXon estimation methods. Method 1 is the following relation:

$$MXon = 1 / (86400 \times MH \times UW3 \times 23.2 AO4^{0.5})$$

```

.....
172 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
3.944012E-09
Documentation: MXon, default file, see file9.nci for basis of data.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection:: 4

MXon is a reciprocal volume/day of air that mixes with pollutant vapor
diffusing into outside air at an onsite location. MXon has the same meaning
as the dispersion term 'CHI/Q'. NOCH3 has two methods to estimate MXon.
Method 1: MXon = 1/(86400*MH*UW3*23.2 AO4^0.5); all input data are online.
In method 2, MH is estimated from AO4; (see User Manual Section 6.4.2).
The MXon value in DEFAULT.LDS is 3.94e-9 day/m^3, based on method 1 with
DEFAULT.LDS MH, UW3, and AO4 input data. Users can input a more elaborate
dispersion model result expressed in day/m^3 units.

.....
172 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
3.944012E-09
Documentation: MXon, default file, see file9.nci for basis of data.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection:: 5
***** Estimation methods for MXon *****
Select '1' for 'box model' with file-supplied mixing height
Select '2' for 'box model' with computed mixing height
Enter your selection:: 2

158 AO4, area of site for outside diffusion/infiltration, ha = 10
151 UW3, wind-speed for on-site exposure to diffusing vapors, m/sec = 2
.....
172 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
1.880886E-09
Documentation: MXon, default file, see file9.nci for basis of data.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection:: 5
***** Estimation methods for MXon *****
Select '1' for 'box model' with file-supplied mixing height
Select '2' for 'box model' with computed mixing height
Enter your selection:: 1

158 AO4, area of site for outside diffusion/infiltration, ha = 10
151 UW3, wind-speed for on-site exposure to diffusing vapors, m/sec = 2
160 MH, rep. mixing height, on-site, m = 20
.....
172 MXon, dilution air factor for vapor flux to outside on-site, day/m^3 =
3.944012E-09
Documentation: MXon, default file, see file9.nci for basis of data.
Main input variable to intake pathway eqtn.
Select '1' to accept current value and documentation message.
Select '2' to replace value
Select '3' to change documentation message
Select '4' to get info message about variable
Select '5' to access estimation method routine. Input selection::

```

Figure 10. Sample Display and Processing Sequence for MXon in NOCH3

The term 86400 converts from seconds (used in UW3) to days. The term  $23.2 AO4^{0.5}$  is based on Turner's approximation<sup>4</sup> for the Gaussian horizontal dispersion coefficient (HDC) at the edge of a square uniform source area; if the width of the square is L, the HDC is  $(L)^{0.5}/4.3$ . Here, the width is assumed to be the square root of the contaminated area AO4. The coefficient 23.2 accounts for the denominator and a conversion to meters from (hectares)<sup>0.5</sup>. The MXon estimate is conservative\* since the dispersion term is designed to predict a three-minute time-averaged exposure rather than long-term exposure, and exposed persons are assumed always at the edge of the area downwind from the prevailing wind direction.

Method 2 uses a similar equation, but internally estimates MH. HDC again equals  $23.2 AO4^{0.5}$ . A pseudo-distance in kilometers, Xpd, conceptually the downwind distance from a point source with similar characteristics to the area source, is back-computed from the C stability curve for the downwind distance-HDC.\*\* The relation is  $Xpd = (HDC/105)^{1.11}$ . Next, a vertical dispersion coefficient (VDC) is computed from an approximate Xpd - VDC relation for C stability curve:  $VDC = 60 Xpd^{0.9}$ . VDC is used in place of MH. This method is subject to the assumptions stated above for the first method. The C stability condition is selected since most on-site exposure is expected to occur during daytime hours.

#### 6.4.3 MXof

PHAS3 has two estimation methods. Method 1 is the following relation:

$$MXof = 1 / (86400 \times (\overline{U}/8) \times MH4 \times UW4 \times [DW4 + 23.2 AO4^{0.5}])$$

The term 86400 converts from seconds (used in UW4) to days. The last term is the sum of two lengths. The first length accounts for uniform wind direction in the area of concern. The second length is the VDC discussed above in the MXon method 1. This equation was suggested by McKone<sup>5</sup>. The MXof estimate is conservative since the dispersion term is designed to compute a three-minute time-averaged exposure.

Method 2 does not require MH4. It uses the following Gaussian equation:

$$MXof = 0.316 / (\overline{U} \times 86400 \times UW4 \times VDC \times HDC)$$

where  $VDC \times HDC = 1900 (Xpd + DW4/1000)^{1.6}$ , and Xpd is estimated as

$$Xpd = (23.2 AO4^{0.5}/70)^{1.11}$$

\* The term conservative means that intake computed with the estimated MX-parameter is larger than that which would be computed if the MX-parameter was exactly known. In terms of the estimated MX-parameter, the dispersion length underestimates what would be the true value.

\*\* Turner<sup>4</sup> uses six stability categories (A through F) as parameters to describe prevailing weather conditions for dispersion calculations. Parametric curves are available for dispersion coefficients as a function of distance downwind from a point source. The curves and an explanation of conditions are in Section 3.3 in the Superfund Exposure Assessment Manual.<sup>6</sup> HDC is often referred to as  $\sigma_y$  and VDC as  $\sigma_z$ .



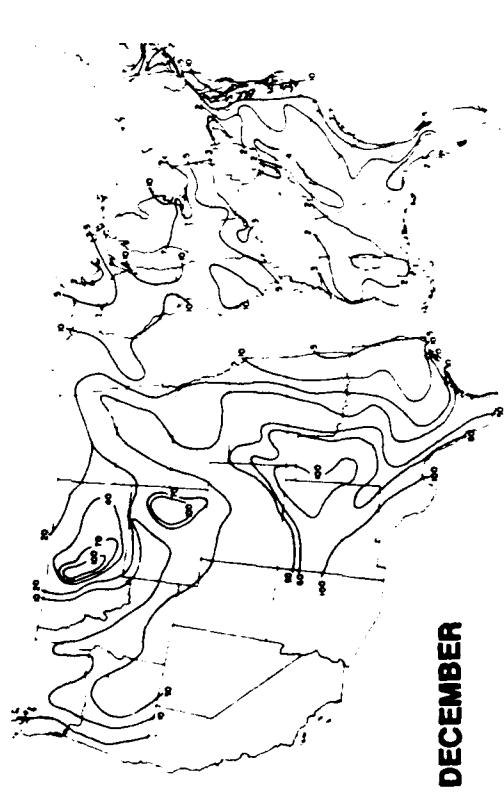
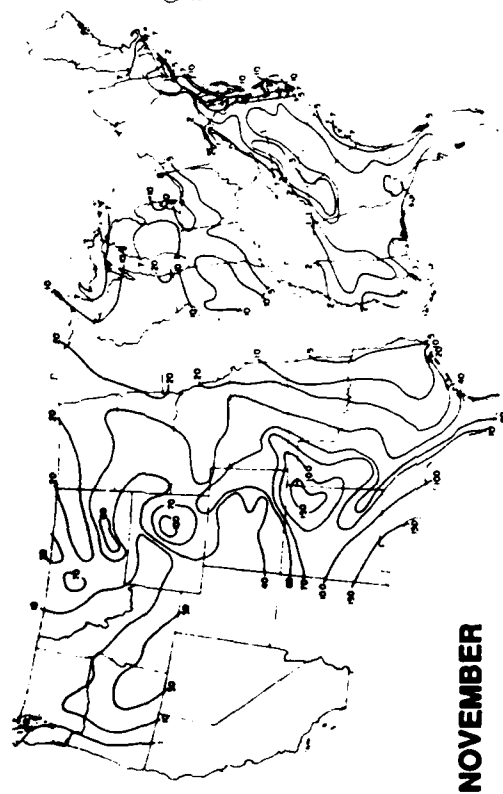
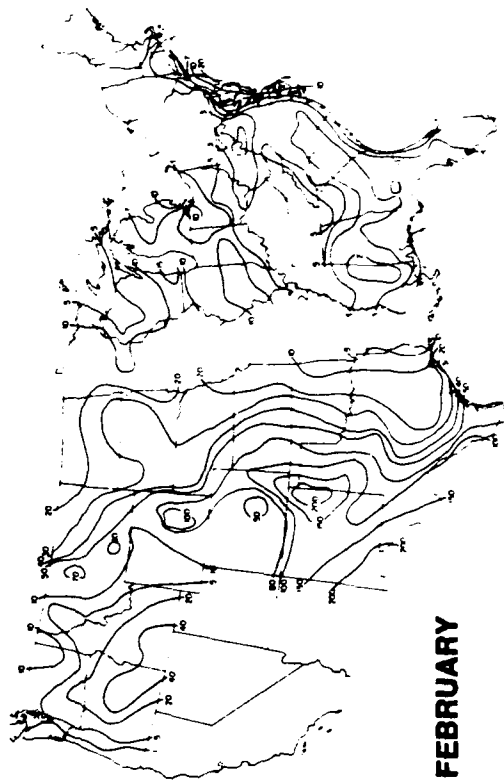
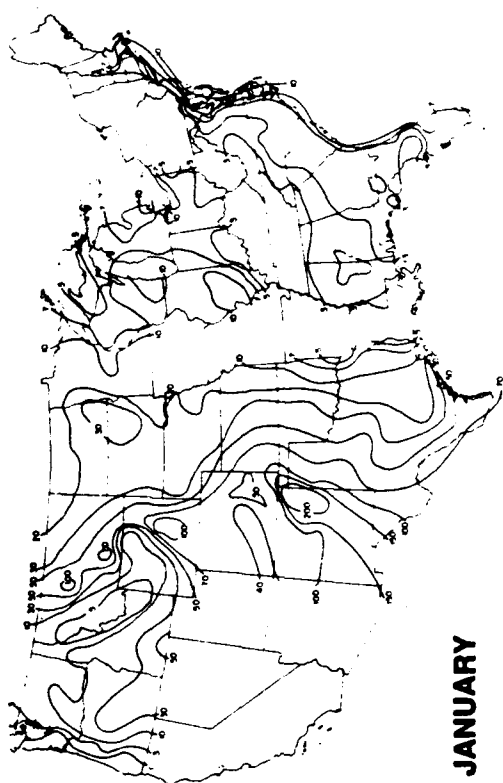
The VDC x HDC product is based on Turner's<sup>4</sup> curves for D stability. The product follows a downwind distance<sup>1.6</sup> power law, and 1900 represents the intercept at 1 km downwind. Here, Xpd is added to the user-provided downwind distance DW4 (input is in meters). Xpd has the same significance as discussed in Section 6.4.2. The back-calculation is based on the D stability curve. The 0.316 attempts to adjust for longer-term dispersion coefficients than those presented by Turner<sup>4</sup>, and is the one-day adjustment that he suggests. This result is conservative, since downwind exposure is always assumed, and D stability dispersion coefficients are usually lower than those expected for exposure during daylight conditions.

#### 6.4.4 MXef

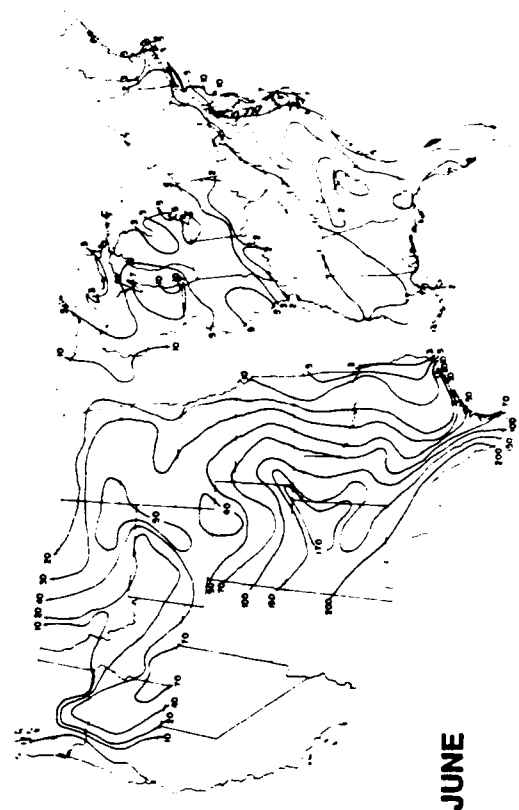
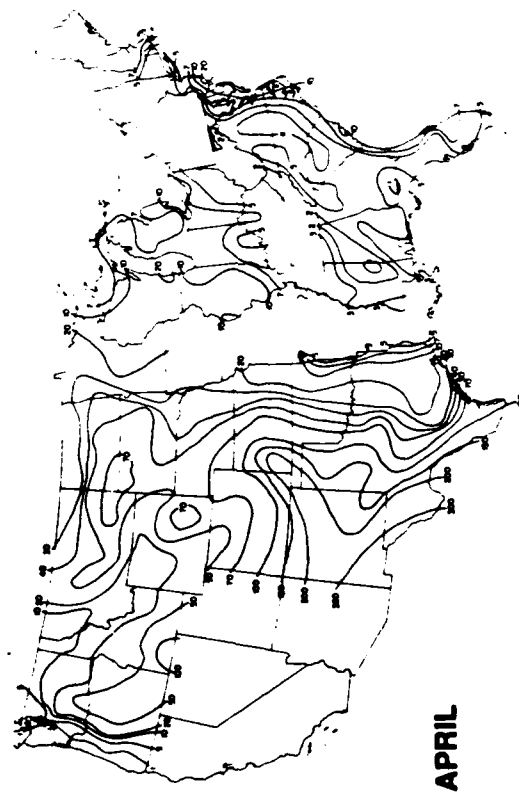
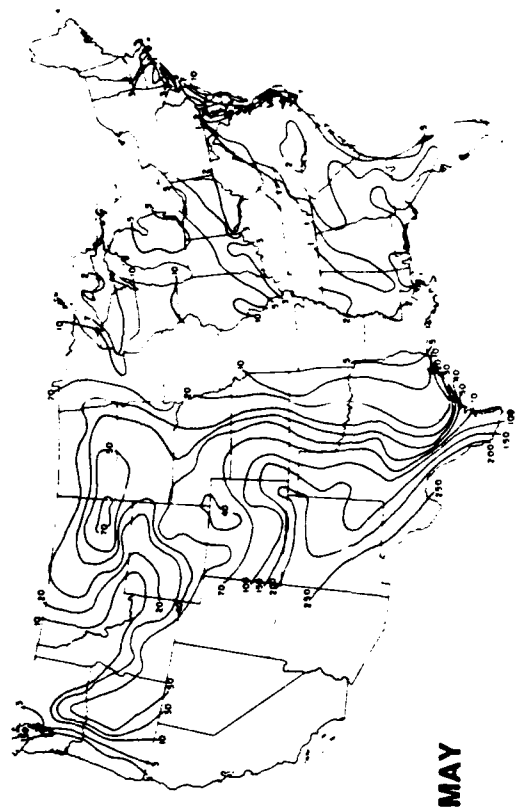
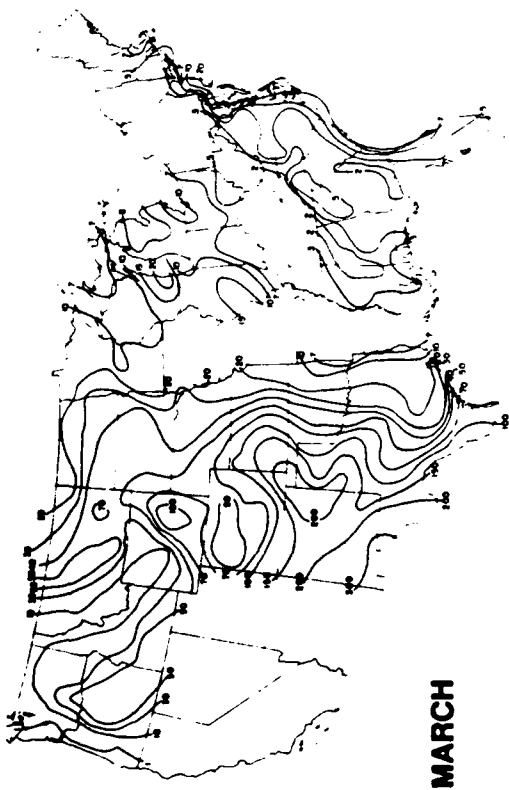
PHAS3 contains one estimation method. The relation used is

$$MXef = 0.133 \times WECF \times 6.1 \times 10^{-4}$$

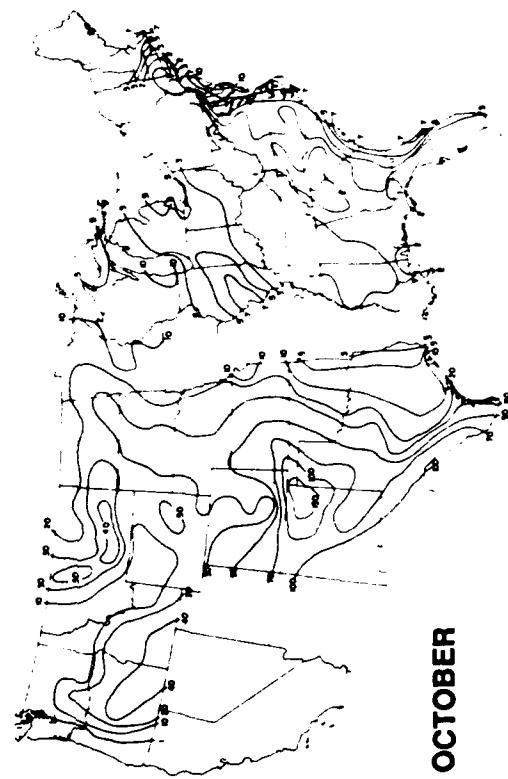
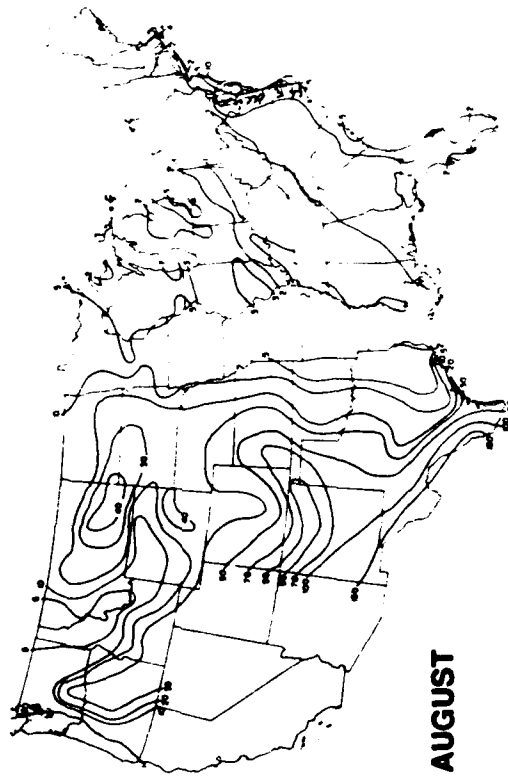
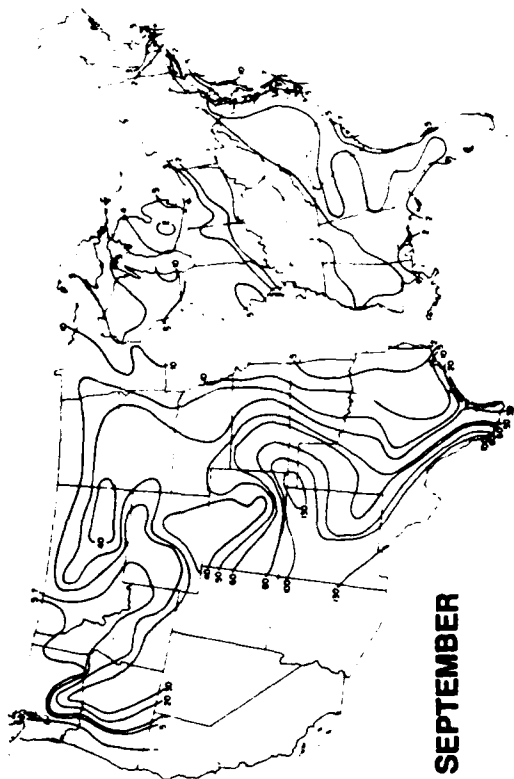
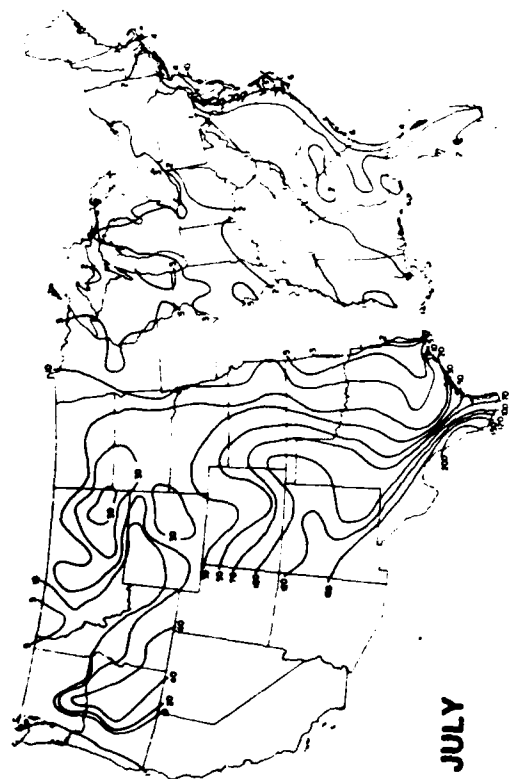
The  $6.1 \times 10^{-4}$  term converts tons/acre-year to  $\text{kg/m}^2\text{-day}$ . The English system term is associated with the 0.133 coefficient. The English system equation was presented by Perry<sup>7</sup>. Figure 11 provides monthly WECF contours for measured values of this parameter at United States locations. These contours are reproduced from Skidmore and Woodruff's paper<sup>8</sup>. WECF can be estimated for each month, and an annual mean computed.



**Figure 11a. WECF Contours by Month: November through February**



**Figure 11b. WECF Contours by Month: March through June**



**Figure 11c. WECF Contours by Month: July through October**

## 7.0 CHMF3

CHMF3 is accessed when '4' is entered at the OPEN3 Main Selection Menu prompt. The initial display is the status report and the main selection menu shown in Figure 12. The status report indicates the last downloaded file, the title of the current online file, the last stored file, and the last file operation with respect to downloaded or stored .DAT files.

There are six functional routines in CHMF3, and the option to exit to OPEN3 without further processing. Several CHMF3 routines resemble those in NOCH3, and in these cases, reference will be made to the last section's descriptions.

### 7.1 Download a .DAT File

The monitor displays the current listing of .DAT files on the Disk 2 device. When prompted, the user specifies a .DAT file to be downloaded. After the file is downloaded, the File Status Report and the CHMF3 Selection Menu reappear for the next function selection; CHMF3 does not have the "load and go" feature of NOCH3. The last line of the status report will read:

"Last file operation was...Downloaded file for further processing"

### 7.2 .DAT File Retrieval, Data Review and Change Procedures

Functions '2', '3' and '4' are discussed here.

#### Obtain the online data from a .DAT file

CHMF3 operates as discussed in Section 6.2, except that .DAT files are being downloaded. In function '4', the file DEFCHEM.DAT is downloaded. Figure 12 shows the display when function '4' is selected.

#### Obtain a DUST

The program operates as discussed in Section 6.2. That section's comments concerning the online status of medium selection and DUST downloaded in NOCH3 also apply in CHMF3.

#### Data Review and Change Routine under DUST CONTROL

A sample display of some routine functions appears in Figure 13. First, the user can change the chemical name information line. This display appears:

Is chemical name: <user supplied information>  
OK? (yes or no)

If the user responds 'yes', the data review and change routine proper begins. If the user responds 'no', this prompt is issued:

Input revised name and other info. (up to 3 lines can be used):

The user can, as is shown in Figure 13, enter a message of up to 255 spaces; see Section 5.4 for input details. If the user wants ONLY to change a title, a "short cut" can be employed. The file NULFIL.PWA is included on Disk 2. This file can be accessed using the procedures in Section 6.2. After title modification, the CHMF3 Selection Menu will be displayed; no other datanames are presented for processing.

```

*** WELCOME TO THE CHEMICAL DATA PROCESSING SUBROUTINE (CHMF3) ***
***** FILE STATUS REPORT *****
Last downloaded file was **
Last stored file was **
Chemical name for online data is **
Last file operation was **
***** CHMF3 MAIN SELECTION MENU *****
ENTER    FUNCTION PERFORMED
  1      Download a stored .DAT file
  2      Modify online information under DUST control.
  3      Modify a stored .DAT file under DUST control.
  4      Create a file for online use or storage.
  5      Go to storage options routine
  6      Modify *online* data via the CRDES3 selection menu.
  0      Exit CHMF3; return to OPEN3.
Enter selection:: 4
This routine will wipeout online .DAT file data. OK (yes/no)?:: yes
File \phas3\disk2\defchem.dat downloaded.
***** CHMF3 DATA USE STATUS TABLE (DUST) LOAD MENU *****
You will need a DUST to process data. Select 1 of 3 options.

```

Figure 12. Initial Display from CHMF3 Main Selection Menu

Data processing follows. As each datum is accessed, its dataname, current value, and current documentation message are displayed. The role of the datum in the assessment is cited; see Section 6.2. Four processing options are provided. The first two options operate as described in Section 6.2. Option '1' starts processing the next dataname selected under DUST control. Option '2' lets the user manually change the existing data value. Option '4' allows the user to change data documentation messages; this process is also shown in Figure 12. Such messages can occupy 255 spaces; Section 5.4 can be consulted for editing specifications.

When option '3' is selected, CHMF3 accesses CRDES3 for a specific subroutine. Below this option's statement line, a message will indicate whether PHAS3 has an informational message only for a given dataname or has a message and estimation method. If an estimation method is employed, the user has the option to either retain the data value online or replace that value with a method estimate (the specific CRDES3 processing is discussed in Section 10.1).

When the data review and change routine is completed, the File Status Report and the CHMF3 Selection Menu reappear and further processing can be done. The last line of the status report is changed and now reads:

Last file operation was...Data change and review routine completed, changes to data (if any) are not stored

### 7.3 .DAT File Storage

The procedures parallel those discussed in Section 6.3, with the substitution of .DAT files for .LDS files. DEFCEM.DAT is not protected against data alternations as is DEFAULT.LDS, but the user is not encouraged to alter it.

### 7.4 Modify Online Data via the CRDES3 Selection Menu

Before this function can be exercised, a .DAT file must be online or the message: " No valid online info, select another option" will appear followed by the CHMF3 Main Selection Menu. If online data are available, CRDES3 is accessed, which is announced by the display of the

```

***** DATA REVIEW AND CHANGE ROUTINE *****
The last file processing action was...
New file set-up routine based on DEFCHEM.DAT
Is chemical name:
2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
OK? (yes or no)::no
Input revised name & other info. (up to 3 lines can be used):: This is where yo
u would place information about the chemical for the .DAT database. As with tit
les and documentation in previous programs, 255 alphanumeric spaces are availabl
e to the user. The use of 255 spaces is shown here, more input is truncated.
***** CHMF3 DUST CONTROL OF DATA PROCESSING ROUTINE *****
176 DTol, Long term limit dose estimate, oral basis, mg/kg-day = .001
Documentation: space for documentation in .DAT File item 176
Main input variable to intake pathway eqtn.
Select '1' to accept current value.
Select '2' to replace value
Select '3' to directly access dataname info/estimation subroutine.
Informational message only available
Select '4' to replace documentation message
Enter your selection:: 2
Enter revised value:: ? .0004

***** CHMF3 DUST CONTROL OF DATA PROCESSING ROUTINE *****
176 DTol, Long term limit dose estimate, oral basis, mg/kg-day = .0004
Documentation: space for documentation in .DAT File item 176
Main input variable to intake pathway eqtn.
Select '1' to accept current value.
Select '2' to replace value
Select '3' to directly access dataname info/estimation subroutine.
Informational message only available
Select '4' to replace documentation message
Enter your selection:: 4
Enter revised documentation message:: This is where you would document the
specific dataname's value.

***** CHMF3 DUST CONTROL OF DATA PROCESSING ROUTINE *****
176 DTol, Long term limit dose estimate, oral basis, mg/kg-day = .0004
Documentation: This is where you would document the specific dataname's value.
Main input variable to intake pathway eqtn.
Select '1' to accept current value.
Select '2' to replace value
Select '3' to directly access dataname info/estimation subroutine.
Informational message only available
Select '4' to replace documentation message
Enter your selection:: 1

***** CHMF3 DUST CONTROL OF DATA PROCESSING ROUTINE *****
177 DTos, Short term limit dose estimate, oral basis, mg/kg-day = .01
Documentation: space for documentation in .DAT File item 177
Main input variable to intake pathway eqtn.
Select '1' to accept current value.
Select '2' to replace value
Select '3' to directly access dataname info/estimation subroutine.
Informational message only available
Select '4' to replace documentation message
Enter your selection::

```

Figure 13. Sample Processing Sequence, CHMF3 Data Review and Change Routine

selection menu shown in Figure 14. The user enters the code number to accesses a specific estimation method routine. The routines are discussed in Sections 10 and 11. Here, the CRDES3-CHMF3 return interface is discussed.

An example of this interface is shown in Figure 31 (Section 11.2). After an estimation method accessed by CRDES3 is completed, the user can replace the online value with the estimation method result. The prompt (in CRDES3) is:

Replace online value with estimate? (yes/no)::

In most cases, after the user's response, this display appears:

\*\* CRDES3 Central Processor: Wish to do more in CRDES3?

Enter 'yes' or 'no'::

If the response is 'yes', the CRDES3 selection table is again displayed. The exception to this display occurs if item 29, 30, 31, or 32 was selected from the CRDES3 Selection Menu (Figure 14). These selections handle two or more datanames. In this case, the display shown is:

\*\* CRDES3 Central Processor: Wish to do more in CRDES3?

CAUTION! If you enter 'yes' and select a different dataname, you cannot change replaced value documentation in CHMF3

Enter 'yes' or 'no'::

If the response is 'no', there is a short pause as the user is transferred back to CHMF3. This return is announced by this display:

\*\*\*\*\* YOU HAVE RETURNED TO CHMF3 \*\*\*\*\*

Current value for <dataname> is <dataname value>

current documentation message: <user-provided message>

---

\*\*\*\*\* CRDES3 SELECTION MENU OF DATA DESCRIBED AND ESTIMATED \*\*\*\*\*

The chemical-related data selected may require data inputs which may also need to be estimated. Consult the user's guide. [D] = description available only. \* = selection of specific datum occurs in estimation routine.

TOXICITY LIMITS	DIFFUSION COEFFICIENTS	SUPER PART. COEFFICIENTS
1-DTol & DTos [D]	16-Da (mol.diff. air)	29-MKrol/MKro2 (soil
2-DTil & DTis [D]	17-Dw (mol.diff. H2O)	runoff model p.c.)
3-DTdl & DTds [D]	18-Kh (Henry's Law const.)	30-MKdb/MKdo (soil
BASIC PHYS PROPS	19-PC (derm. perm. const.)	vapor model p.c.)
4-MW (mol weight)[D]	PARTITION COEFFICIENTS	31-MKgw (soil infil.
5-Tm (melt point)[D]	20-BAF (fish bioacc. factor)	to groundwater p.c.)
6-Tb (boiling point)	21-Kwv (H2O->veg p.c.)	32-MKdw (sediment->
7-LogP (oct.-H2O p.c.) [D]	22-Kwp (H2O->plant p.c.)	water diffusion p.c.)
8-Wsol (water sol.)	23-Kpm (plant->meat p.c.)	CONSTRAINT INPUTS
9-VP (Sat. vapor press.)	24-Kpd (plant->dairy p.c.)	33-Organoleptic[D]
PARTITION COEFF INPUTS	25-Kd (soil->water p.c.)	34-Aquatic tox [D]
10-Koc (OC->water p.c.)	PERSISTENT RATE CONSTANTS	35-Phytoxox [D]
11-Ksv (Soil->veg. p.c.)	26-LPwat (in water)[D]	36-Livestock tox.[D]
12-Ksp (Soil->forage p.c.)	27-LPsed (in sediment)[D]	TIME ADJUSTMENTS
13-Ref. foc for Ksv&Ksp[D]	28-LPsoils (3 choices)[D]	37-Tox limit adjust.[D]
14-Kpat(plant->ad.tiss.p.c.)		
15-BCF (Fish bioconc. factor)		

Select '0' to quit without selection

Input the subroutine selection number::

Figure 14. CRDES Selection Menu Accessed from CHMF3 via. Function '6'



If an online value was replaced by the user, after re-entry to CHMF3, the user can document a replaced value. The following is displayed

"Do you want to change documentation (yes/no)?::"

With a yes response, the next prompt is: "Enter revised documentation message::"

After revised documentation is entered, the CHMF3 Main Selection Menu appears.

If an online value is NOT replaced in CRDES3, when the user exits CRDES3, the CHMF3 Main Selection Menu appears next. This menu also appears after the user responds 'no' to the "Do you want to change documentation" prompt.

## 7.5 Chemical-Related Data File Structure

The user should be aware of the chemical-related data order and features of CRDES3 to avoid "surprises" in estimation method subroutines. The data in a .DAT file are indexed from 176 to 250; see Table 3. The indices 176-185 are reserved for toxicological data. The indices 186-191 are reserved for conventional physical properties of substances. The datanames indexed from 206-219 and from 231-240 are used in at least one pathway or route intake equation. The data index is sequenced so that data intended as inputs to specific estimation subroutines are obtained before the subroutine is executed. As examples, some vapor pressure estimation methods require boiling point data as input; some fish bioconcentration factor estimation methods require the octanol-water partition coefficient as input.

When data review and change are under DUST control, the index order ensures that input data to estimation methods are available. When function '6' is selected, the user assumes this responsibility. Two features assist the user:

- o The Scenario Data Needs Report presents datanames in index order, and provides guidance as to what data inputs are required for specific methods.
- o The CRDES3 Selection Menu is ordered such that the most fundamental data are listed first.

The estimation methods for datanames indexed from 213 to 240 involve non-chemical data inputs, which CRD113 accesses from a .LDS file. Section 11 includes several examples of the accession procedure.

The datanames indexed from 231-240 are model results expressed as partition coefficients (the "super" partition coefficients discussed in Section 2). To stress this, the datanames are prefixed "MK". If their values are manually entered, the user should be clear as to the units expected.

The CRDES3 subroutines for MKdb, MKdo, MKdw and MKgw provide time-averaged estimates, since the methods therein incorporate two mechanisms that diminish pollutant content in the medium source over an exposure time period. Each such period is a non-chemical related datum, and the user must ensure that such data are in the intended .LDS file prior to entry to CRDES3.

Data indexed from 241-247 are reserved for inputs to the Type 1 constraint analysis. If these data are not available, or the user does not want to include a constraint in his analysis, a negative data value should be assigned. The negative value serves as a "flag" to omit the constraint. Other .DAT file data should not be assigned a zero value.

## 8.0 DIAG3

DIAG3 is accessed when '5' is entered at the OPEN3 Main Selection Menu prompt. DIAG3 is announced with this menu:

\*\*\*\*\* DIAGNOSTIC UTILITY MENU \*\*\*\*\*

ENTRY	FUNCTION
0	Quit utility and return to OPEN3
1	Display pathway status (SST) for online scenario
2	Display data use status table (DUST) for scenario
3	Display online non-chemical data (.LDS data)
4	Display online chemical-related data (.DAT data)
5	Printout online data (datanames supplied) and documentation
6	Review and change online data and documentation

Enter your selection::

The '0' entry to this menu returns the user to the OPEN3 Main Selection Menu. At the end of any other entry function, the above menu reappears. The subsections below discuss these functions. The information in the figures shown in this Section are related to the problem developed in Section 5.5.

### 8.1 Display Pathway Status (SST) for Online Scenario

The display is shown in Figure 15. The SST is presented in two columns, each under a "Paths" heading. The left column contains a coded entry for pathways (or routes) from 1 to 10; the rightmost column, for pathways 11 to 20. The pathway or route - column location correspondence appears in Table 4. The asterisks in Table 4 indicate pathways in the sample problem. If the entry for a pathway is zero, the pathway (route) is not included in the scenario. For sediment pathways, the coded entry is the same as the location number in Table 4. For the surface water or groundwater pathways 1 through 8, the pathway location is the code number. If pathway 9 is included, and the option is water intake by livestock, the code listed is "9". Otherwise, (water and plant intake by livestock option) it is "10". If pathway 10 is included, the corresponding codes are "11" and "12".

TABLE 4. PATHWAY (ROUTE) LOCATION NUMBER FOR SST DISPLAY IN DIAG3

#### Left Column

Domestic water ingestion (1)\*  
Inhalation of vapors from domestic water(2)\*  
Domestic water dermal absorption (3)\*  
Water recreation\ water ingestion (4)  
Water recreation\ vapor inhalation (5)  
Water recreation\ dermal absorption (6)  
Fish consumption (7)  
Vegetable consumption (8)\*  
Beef consumption (9)\*  
Milk consumption (10)

#### Right Column

Dust intake in vicinity of on-site residence (11)\*  
Dust intake at an on-site work setting (12)  
Inhaled vapors diffused from soil in house (13)\*  
Inhaled vapors diffused from soil at on-site location (14)\*  
Inhaled vapors diffused from soil at off-site location (15)  
Domestic water-groundwater supply\ ingestion (16)  
Domestic water-groundwater supply\ vapor inhalation (17)  
Domestic water-groundwater supply\ dermal absorption (18)

```

5   Printout online data, datanames supplied
6   Review specific data name/value with option to
    change online data.
Enter your selection: 1
      Paths 1-10  Paths 11-20
1         0         26
2         0         0
3         0         29
4         0         0
5         0         0
6         0         0
7         0         0
8        12         0
9        19         0
10        0         0

Read down column for pathway status: 0 = not used
Online scenario title is: Sample problem for manual
Environmental medium of scenario is... Surface and near-surface soil pathways
Last downloaded file was ... ptsample.pts
Last stored file was... ptsample.pts
If no downloaded or stored file shown above, data is only online
Last file processing was... New SST/DUST stored on Disk 2 device file.
Hit enter (return) to continue....

```

Figure 15. DIAG3 Display of SST for PTSAMPLE.PTS

For the surface and near surface soil pathways, the relation of code to SST display location is more complex, and is shown below:

Code	Location	Subsite/Option
1 through 3	1 through 3	Respectively, no options
4 or 5	4	Subsite 1 or 2 respectively
6 or 7	5	Subsite 1 or 2 respectively
8 or 9	6	Subsite 1 or 2 respectively
10 or 11	7	Subsite 1 or 2 respectively
12 or 13	8	Subsite 1 or 2 respectively
14 or 15	9	Plant intake by animal, subsite 1 or 2 respectively
16 or 17	9	Plant + soil intake by animal, subsite 1 or 2 respectively
18 or 19	9	Plant + soil + water intake by animal, subsite 1 or 2 respectively
20 or 21	10	Plant intake by animal, subsite 1 or 2 respectively
22 or 23	10	Plant + soil intake by animal, subsite 1 or 2 respectively
24 or 25	10	Plant + soil + water intake by animal, subsite 1 or 2 respectively
26	11	Subsite 1
27	12	Subsite 2
29 through 34	13 through 18	Respectively

After the code display in Figure 15, the following narrative appears:

```

Read down column for pathway status: 0 = not used
Online scenario title is ....<title supplied by user for .pxx file>
Environmental medium of scenario is <medium selected by user>
Last downloaded file was...<filename + .pxx extension, if any>
Last stored file was...<filename + .pxx extension, if any>
If no download or stored file shown above, data is only online
Last file processing was...<statement of last operation in PATWAY3>

```

If this function is accessed without a valid SST, all location number entries will be zero, and bracketed terms will be blank.

## 8.2 Display Data Use Status Table (DUST) for a Scenario

The PTSAMPLE.PTS DUST display is in Figure 16. After the first part of the table is displayed, the user responds to the "Hit enter (return) to continue..." prompt to display the rest of the table. The first part shows the DUST code for the first 120 datanames; the second part, for the last 130 datanames. Each line has ten columns of index numbers. The numbers are read from left to right and then down. Thus, the right-most index number in the first row is the DUST code of the index '10' datum (adult vegetable consumption). For other data, the table is read down to the tens position and then across to the units position. The DUST code entries are integers from "0" to "7", and correspond to these statements:

- 0 The datum is not needed.
- 1 The datum is used in at least one exposure pathway equation.
- 2 The datum is used to estimate other data that appear in at least one exposure pathway equation.
- 3 Both statements 1 and 2 apply
- 4 The datum is used in a constraint equation.
- 5 Both statements 1 and 4 apply.
- 6 Both statements 2 and 4 apply
- 7 Both statements 2 and 5 apply

As an example in Figure 16, the DUST index for the datum with index 211, the water to vegetable partition coefficient, Kwv, is '7'. Thus, this coefficient could be used in three different ways in the example scenario, as indicated by statements 1, 2, and 4.

#ten	#ten+1	#ten+2	#ten+3	#ten+4	#ten+5	#ten+6	#ten+7	#ten+8	#ten+9	#ten+10
0	1	0	0	0	0	0	0	0	0	1
1	1	0	1	1	1	1	0	1	0	0
2	0	0	0	0	0	1	0	0	0	0
3	0	0	0	0	1	1	0	1	1	1
4	1	0	1	0	0	0	0	0	0	0
5	1	1	0	0	0	0	0	0	0	0
6	0	0	1	1	0	0	0	0	0	0
7	0	0	0	0	0	0	3	3	0	0
8	0	0	0	0	0	2	2	5	5	5
9	4	4	4	4	4	0	0	0	0	0
10	0	0	0	0	0	0	0	0	0	0
11	2	5	5	0	0	0	0	0	0	0
12	0	0	0	2	0	2	7	7	2	2

To locate DUST entry index, read down 'tens' column, then across.

Hit enter (return) to continue....

13	2	2	2	2	2	2	2	2	0	0
14	2	2	2	2	2	2	2	1	0	0
15	0	0	0	0	0	0	0	0	0	0
16	0	0	0	0	0	0	0	0	0	0
17	1	0	0	0	0	1	1	1	1	1
18	1	0	0	0	1	2	2	2	2	2
19	2	2	2	2	2	2	2	0	0	0
20	0	0	0	0	0	2	0	2	0	0
21	7	7	1	2	5	7	2	0	0	0
22	0	0	1	1	2	0	0	0	0	0
23	0	5	1	1	0	0	0	0	0	0
24	4	0	4	4	4	4	4	0	0	0

To locate DUST entry index, read down 'tens' column, then across.

Hit enter (return) to continue....

Figure 16. DIAG3 Display of DUST for PTSAMPLE.PTS

### 8.3 Online Data Displays

Non-chemical data can be reviewed by responding with '3' to the Diagnostic Utility Menu. Figure 17 shows the two-screen display for DEFAULT.LDS. The data are read from left to right in each row. The first row entry indicates the base number. In the row with base "90+", the value 16.6 under the column "two" is for the dataname with index 92 (Upd). The first screen shows data indexed from 1 to 100. The second screen shows data indexed from 101 to 175. These listings are followed by a narrative indicating the title line for the online data, the name of the last downloaded .LDS file, the last file to which data were stored (if any), and the last .LDS file operation performed.

Chemical-related data can be reviewed by responding with '4' to the Diagnostic Utility Menu. Figure 18 shows this display for DEFCHEM.DAT. The location of indices is that discussed above. The data table is concluded by a narrative which follows the sequence cited above for .LDS files.

```

Data for Non Chemical Data index from 1 to 100
For location, read down side for index multiple of 5, then across
line   one      two      three     four      five
0 +    70      1.6      3.4      1.8      .3
5 +    8.999999E-03 .45      .18      .0065     .017
10 +   .044      .18      .0001     .52      .35
15 +   13      .0004     1.5      15      0
20 +   0        0        0        0        0
25 +   13      .5       1.05     .6       .3
30 +   8.999999E-03 .18      .18      .0022     .007
35 +   .02      .56      .0002     .26      .35
40 +   5.1      0        .63      5.7      0
45 +   0        0        0        0        0
50 +   .0145     7E-08    .37      2        .3
55 +   0        0        0        0        0
60 +   .95      .95      .95      .95      .95
65 +   .95      0        0        0        0
70 +   0        0        0        7300     10950
75 +   365      10950    365      10950    365
80 +   0        0        0        0        0
85 +   .2       .04      15.3     6.6      .35
90 +   78      16.6     .87      250      520
95 +   0        0        0        0        0
Hit enter (return) to continue....

```

```

For location, read down side for multiple of 5, then across.
line   one      two      three     four      five
100 +  .04      1.5      .4       .5       5
105 +  100      1        0        0        0
110 +  .02      1.4      .1       10       100
115 +  .08      .25     .35      1        .12
120 +  1        8        .2       150      0
125 +  .03      1.4      .1       20       100
130 +  .08      .25     .35      1        .12
135 +  1        10       .2       0        0
140 +  .003     1.8      .15      .2       .1
145 +  3        2400    125      0        0
150 +  2        .003     1.8      .15      .2
155 +  .1       5        10       2        20
160 +  500      30       10       .1       365
165 +  10      .35      0        0        0
170 +  .000417  3.94E-09 5.5E-10 .0000162 0
Title assigned from downloaded/online file is:
Default file for starting new .LDS file. Check user's guide for parameter value
derivation.
Last downloaded file was ...default.lds
Data stored in...
Last file operation... Downloaded 'to go' file
Hit enter (return) to continue....

```

Figure 17. DIAG3 Display of Database in DEFAULT.LDS

#### 8.4 Printout Online Data (Datanames Supplied) and Documentation

As a precaution, if any online data documentation has been changed in the current DIAG3 session (see Section 8.5), this message is issued:

Answer 'yes' or 'no'

You may have changed online data documentation

Do you want these changes to appear in printout?::

If the response is "no", all documentation changes (but not data changes) made in the current DIAG3 session are wiped out. If there have been no such documentation changes, the program checks for downloaded .LDS and .DAT files. If either type file has not been downloaded, a message with format:

WARNING! You have not downloaded a <non-chemical> <chemical-related> data file is issued for each missing type file. In such a situation, printouts requested will report zeroes for datanames involved in missing files.

The following menu is displayed:

```
ENTER      OPTION
0          For no printout, return to Diagnostic Utility Menu
1          Printout ALL data online
2          Printout ALL SCENARIO-RELATED data
3          Printout ONLY data used in intake/constraint equations
All printouts will include data documentation messages
Enter your selection here::
```

Respond '0' to exit this routine. The other entries cause a printout of datanames followed by their online values and documentation. The extent of the printout is governed by the response entry. If the response is '1', the printout includes all datanames which are used in PHAS3 regardless of their use in the online scenario. If the response is '2', the printout includes any

line	one	two	three	four	five
175 +	.001	.01	.001	.01	.0001
180 +	.0001	0	0	0	2
185 +	227	25.32	2.32	.001	303
190 +	.0004	1000	.02	.2	.02
195 +	.02	.005	200	0	0
200 +	0	0	0	0	0
205 +	.55	.000055	.00003	.0008	210
210 +	1.5	15	.001	.0002	20
215 +	10	2	5	50	0
220 +	.01	.001	.1	.1	.00001
225 +	0	0	0	0	0
230 +	1765.728	11111	390.9059	50	100
235 +	200	1567.391	1550	500	1000
240 +	.01	-1	.05	5	20
245 +	.015	.01	0	0	0

For location, read down side for multiple of 5, then across.

Data is for substance...

2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...

Last downloaded file was...defchem.dat. Data stored in ...

Last file operation... Downloaded file for further processing

Hit enter (return) to continue....

Figure 18. DIAG3 Display of Database in DEFCHEM.DAT

datanames with a non-zero entry in the DUST. If the response is '3', the printout includes only those data that appear either in intake equations in COMP3 or in the constraint equations. Figure 19 is the option '3' printout of datanames, values, and documentation in DEFAULT.LDS and DEFCHEM.DAT with the sample problem DUST. The printout concludes with the title lines for the scenario, the non-chemical data file, and the chemical-related data file.

If '2' or '3' is entered, and a DUST is missing or defective, the message  
DUST either not available or defective  
is issued, and the user is returned to the Printout Options Menu.

### 8.5 Review and Change Online Data and Documentation

The routine checks if non-chemical and chemical-related data are online. If either set is not online, one or two caution messages in this format appear:

WARNING! You have not downloaded a <non-chemical> <chemical-related> data file

The routine will operate; values of zero and blank documentation fields are displayed. User inputs start with this menu:

\*\*\*\*\* ONLINE DATA REVIEW AND CHANGE ROUTINE \*\*\*\*\*

CAUTION! You must supply dataname index first.

OPTION	FUNCTION PERFORMED
0	Return to DIAGNOSTIC UTILITY menu
1	Review a dataname and value
2	Change the reviewed value
3	Change the documentation message

Enter your selection here::

The entry '0' exits this routine. Option '1' must be selected before any of the other menu options can be done, otherwise this message appears:

You must enter an index number; do this now.

After the entry '1', this prompt appears:

Enter the index number for the datum::

to which the user provides the index (from 1 to 250). One of two messages will appear. If the index is currently not used in PHAS3, the message is:

<index number> not used. Try again.

Otherwise the message is in the form:

The dataname is.... <title line from Table 1>

Its value is:: <data value>

Documentation...<current documentation message>

The menu is again displayed. If option '2' is selected, the user is prompted:

Enter the new datum value::

The user enters a value. The program displays the revised information in the format shown above followed by the option selections.

If option '3' is selected, the user is prompted: "Enter new datum documentation::"

As shown in Figure 20, the documentation can occupy up to 255 spaces; see Section 5.4 for editing specifications.

Figure 20 presents a display sequence that demonstrates this routine's functions. Online databases with altered data and documentation can be stored to the disk 2 device in NOCH3 and CHMF3.

1 Bwa, adult body weight, kg ,70  
 Documentation: Bwa, default file, see file1.nci for basis of data.  
 10 Wva, adult vegetable consumption, kg dwb/day ,.017  
 Documentation: Wva, default file, see file1.nci for basis of data.  
 11 Wma, adult beef consumption, kg/day ,.044  
 Documentation: Wma, default file, see file1.nci for basis of data.  
 13 SIRa, adult oral intake of soil, residential, kg/day,.0001  
 Documentation: SIRa, default file, see file1.nci for basis of data.  
 14 SARA, adult exposure area to dust on skin, residential, m<sup>2</sup>,.52  
 Documentation: SARA, default file, see file1.nci for basis of data.  
 15 PLa, adult perspiration rate, L/m<sup>2</sup>/day,.35  
 Documentation: PLa, default file, see file1.nci for basis of data.  
 16 OIRa, adult inhalation rate, onsite residential, m<sup>3</sup>/day,13  
 Documentation: OIRa, default file, see file1.nci for basis of data.  
 18 BIRa, adult inhalation rate, basement vapors, m<sup>3</sup>/day,1.5  
 Documentation: BIRa, default file, see file1.nci for basis of data.  
 26 BWc, child body weight, kg ,13  
 Documentation: BWc, default file, see file2.nci for basis of data.  
 35 Wvc, child vegetable consumption, kg/day ,.007  
 Documentation: Wvc, default file, see file2.nci for basis of data.  
 36 Wmc, child beef consumption, kg/day ,.02  
 Documentation: Wmc, default file, see file2.nci for basis of data.  
 38 SIRc, child oral intake of soil, residential, kg/day,.0002  
 Documentation: SIRc, default file, see file2.nci for basis of data.  
 39 SARc, child exposure area to dust on skin, residential, m<sup>2</sup>,.26  
 Documentation: SARc, default file, see file2.nci for basis of data.  
 40 PLc, child perspiration rate, L/m<sup>2</sup>/day,.35  
 Documentation: PLc, default file, see file2.nci for basis of data.  
 41 OIRc, child inhalation rate, onsite residential, m<sup>3</sup>,5.1  
 Documentation: OIRc, default file, see file3.nci for basis of data.  
 43 BIRc, child inhalation rate, basement vapors, m<sup>3</sup>/day,.63  
 Documentation: BIRc, default file, see file3.nci for basis of data.  
 51 SLA, soil loading rate on exposed skin, kg/m<sup>2</sup>/day,.0145  
 Documentation: SLA, default file, see file3.nci for basis of data.  
 52 RSPA, particulate conc in air, residential, kg/m<sup>3</sup> ,7E-08  
 Documentation: RSPA, default file, see file3.nci for basis of data.  
 63 AFta, Time adjustment factor, long-term (adult), topsoil paths,.95  
 Documentation: AFIt, default file, see file4.nci for basis of data.  
 64 AFtc, Time adjustment factor, short-term (child), topsoil paths,.95  
 Documentation: AFst, default file, see file4.nci for basis of data.  
 77 TEta, Time exposure for adult, topsoil pathways, days,10950  
 Documentation: TEtl, default file, see file4.nci for basis of data.  
 78 TEtc, Time exposure for child, topsoil pathways, days,365  
 Documentation: TEts, default file, see file4.nci for basis of data.  
 88 Uwm, water intake by steer, L/day,15.3  
 Documentation: Uwm, default file, see file5.nci for basis of data.  
 89 Upm, plant (forage) intake by steer, kg (dwb)/day,6.6  
 Documentation: Upm, default file, see file5.nci for basis of data.  
 90 Usm, soil intake by steer, kg/day,.35  
 Documentation: Usm, default file, see file5.nci for basis of data.  
 91 Uwd, water intake by dairy cow, L/day,78  
 Documentation: Uwd, default file, see file5.nci for basis of data.  
 92 Upd, plant (forage) intake by dairy cow, kg (dwb)/day,16.6  
 Documentation: Upd, default file, see file5.nci for basis of data.  
 93 Usd, soil intake by dairy cow, kg/day,.87  
 Documentation: Usd, default file, see file5.nci for basis of data.  
 94 BWm, representative steer body weight, kg,250  
 Documentation: BWm, default file, see file5.nci for basis of data.  
 95 BWD, representative dairy cow body weight, kg,520  
 Documentation: BWD, default file, see file5.nci for basis of data.

Figure 19. DIAG3 Printout of Databases from DEFAULT.LDS and DEFCEM.DAT,  
 Option 3 (page 1 of 2 pages)



112 rh1, bulk density, topsoil #1 subsite, kg/L,1.4  
 Documentation: rh1, default file, see file6.nci for basis of data.  
 113 th1, average moisture capacity, topsoil #1 subsite, L/L,.1  
 Documentation: th1, default file, see file6.nci for basis of data.  
 127 rh2, bulk density, topsoil #2 subsite,1.4  
 Documentation: rh2, default file, see file7.nci for basis of data.  
 128 th2, average moisture capacity, topsoil #2 subsite, L/L,.1  
 Documentation: th2, default file, see file7.nci for basis of data.  
 148 Ab3, basement area contacting soil diffusing vapors,m<sup>2</sup>,125  
 Documentation: Ab3, default file, see file8.nci for basis of data.  
 171 MXb, dilution air factor for vapor flux in basement, day/m<sup>3</sup>,.000417  
 Documentation: MXb, default file, see file9.nci for basis of data.  
 176 DTol, Long term limit dose estimate, oral basis, mg/kg-day,.001  
 Documentation: space for documentation in .DAT File item 176  
 177 DTos, Short term limit dose estimate, oral basis, mg/kg-day,.01  
 Documentation: space for documentation in .DAT File item 177  
 178 DTil, Long term limit dose estimate, inhalation basis, mg/kg-day,.001  
 Documentation: space for documentation in .DAT File item 178  
 179 DTis, Short term limit dose estimate, inhalation basis, mg/kg-day,.01  
 Documentation: space for documentation in .DAT File item 179  
 180 DTdl, Long term limit dose estimate, dermal basis, mg/kg-day,.0001  
 Documentation: space for documentation in .DAT File item 180  
 181 DTds, Short term limit dose estimate, dermal basis, mg/kg-day,.0001  
 Documentation: space for documentation in .DAT File item 181  
 185 TAF, Long term averaging time adjustment code,2  
 Documentation: space for documentation in .DAT File. Enter 1 if known/suspected  
 211 Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L,1.5  
 Documentation: space for documentation in .DAT File item 211  
 212 Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L,15  
 Documentation: space for documentation in .DAT File item 212  
 213 Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb),.001  
 Documentation: space for documentation in .DAT File item 213  
 215 Kd1 soil/water p.c. for #1 subsite pathways, mg/kg / mg/L,20  
 Documentation: space for documentation in .DAT File item 215  
 216 Kd2 soil/water p.c. for #2 subsite pathways, mg/kg / mg/L,10  
 Documentation: space for documentation in .DAT File item 216  
 223 LPts1, persistence rate constant for #1 subsite soil, 1/year,.1  
 Documentation: space for documentation in .DAT File item 223  
 224 LPts2, persistence rate constant for #2 subsite soil, 1/year,.1  
 Documentation: space for documentation in .DAT File item 224  
 232 MKro2, model soil-water p.c., #2 subsite runoff, mg/kg / mg/L,11111  
 Documentation: space for documentation in .DAT File item 232  
 233 MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m<sup>2</sup>-day,390.9  
 Documentation: space for documentation in .DAT File item 233  
 234 MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m<sup>2</sup>-day,50  
 Documentation: space for documentation in .DAT File item 234  
 241 TOL, Organoleptic limit - taste in water, mg/L,.01  
 Documentation: space for documentation in .DAT File item 241  
 243 AQTL, Aquatic toxicity limit in water, mg/L,.05  
 Documentation: space for documentation in .DAT File item 243  
 244 PHLW, Phytotoxicity limit in water, mg/L,5  
 Documentation: space for documentation in .DAT File item 244  
 245 PHLS, Phytotoxicity limit in soil, mg/kg,20  
 Documentation: space for documentation in .DAT File item 245  
 246 focPS, foc for soil used to determine phytotoxicity limit,.015  
 Documentation: space for documentation in .DAT File item 246  
 247 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day,.01  
 Documentation: space for documentation in .DAT File item 247  
 Substance is 2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for somethin  
 Site data tile is: Default file for starting new .LDS file. Check user's guide  
 Scenario title is: Sample problem for manual

Figure 19. DIAG3 Printout of Databases from DEFAULT.LDS and DEFCHEM.DAT,  
 Option 3 (page 2 of 2 pages)

Enter your selection:: 6  
 WARNING! You have not downloaded a chemical-related data file.  
 \*\*\*\*\* ONLINE DATA REVIEW AND CHANGE ROUTINE \*\*\*\*\*  
 CAUTION! You must supply dataname index first.

OPTION	FUNCTION PERFORMED
0	Return to DIAGNOSTIC UTILITY menu
1	Review a dataname and value
2	Change the reviewed value
3	Change the documentation message

Enter your function number::2  
 You must enter an index number; do this now.  
 Enter the index number for the datum::92  
 The dataname is....  
 92 Upd, plant (forage) intake by dairy cow, kg (dwb)/day  
 Its value is:: 16.6  
 Documentation... Upd, default file, see file5.nci for basis of data.

OPTION	FUNCTION PERFORMED
0	Return to DIAGNOSTIC UTILITY menu
1	Review a dataname and value
2	Change the reviewed value
3	Change the documentation message

Enter your function number::2  
 Enter the new datum value::17.7  
 The dataname is....  
 92 Upd, plant (forage) intake by dairy cow, kg (dwb)/day  
 Its value is:: 17.7  
 Documentation... Upd, default file, see file5.nci for basis of data.

OPTION	FUNCTION PERFORMED
0	Return to DIAGNOSTIC UTILITY menu
1	Review a dataname and value
2	Change the reviewed value
3	Change the documentation message

Enter your function number::3  
 Enter new datum documentation::This is the new data message for this dataname.  
 As with other documentation and titles in PHAS3, this documentation can occupy up  
 to 255 spaces. Your input in excess of 255 spaces is truncated by BASIC. This  
 message occupies 255 spaces.  
 The dataname is....  
 92 Upd, plant (forage) intake by dairy cow, kg (dwb)/day  
 Its value is:: 17.7  
 Documentation...  
 This is the new data message for this dataname. As with other documentation and  
 titles in PHAS3, this documentation can occupy up to 255 spaces. Your input in e  
 xcess of 255 spaces is truncated by BASIC. This message occupies 255 spaces.

OPTION	FUNCTION PERFORMED
0	Return to DIAGNOSTIC UTILITY menu
1	Review a dataname and value
2	Change the reviewed value
3	Change the documentation message

Enter your function number::

Figure 20. Sample Display of DIAG3 Data Review and Change Routine

## 9.0 ASSESSMENT AND CONSTRAINT ANALYSIS PROGRAMS

### 9.1 The Public Health Assessment Program, COMP3

COMP3 is accessed when '7' is entered at the OPEN3 Main Selection Menu prompt. This preamble is displayed:

```
***** WELCOME TO COMP3, THE PUBLIC HEALTH ASSESSMENT PROGRAM *****  
COMP3 does the assessment for the SST, non-chemical data set and  
chemical-related data set currently on line. Then you have the option  
to do the constraint analysis. First, a check is made for online information  
and data. If there are problems, they will be identified, and you will be  
sent back to OPEN3 to do further processing as required.
```

If either a .PXX-, .LDS-, or .DAT- type file is missing, this condition will be noted, and after a continuation return, the OPEN3 Main Selection Menu appears. The program then checks intake equation data inputs; if an expected input is zero or less, this message is issued:

```
Missing data indicated for indexed variable <dataname>  
Provide data either in DIAG3 accessed from OPEN3  
in NOCH3 for datanames indexed 1-175, CHMF3 for datanames indexed 176-250
```

After a continuation return, the OPEN3 Main Selection Menu will appear.

If online information and data are in order, the following message appears:

```
You have valid online information and data available. A status  
summary is listed. Then you can choose to continue or not.  
Hit enter (return) to continue....
```

After the continuation return, a summary report on the scenario, non-chemical data and chemical-related data is presented. This report includes the title of the scenario, site information, or chemical in the respective online database. The report states the last files downloaded and stored, and the last data processing operations in PATWAY3, NOCH3 and CHMF3. The user is then queried:

```
Answer yes or no  
Do you wish to continue...
```

If the user responds 'no' at this prompt, COMP3 is exited, and the OPEN3 Main Selection Menu is displayed. This "escape" is provided in case the wrong downloaded file data are online.

If the user responds 'yes' at this prompt, this message is displayed:

```
Ready to begin analysis. If you have not done so already, you  
should consider a printout of display of your database in DIAG3.  
***** ASSESSMENT BASIS (ADULT OR CHILD) SELECTION *****  
Input '1' for adult-based analysis  
Input '2' for child-based analysis  
Input '3' for both analyses:
```

COMP3 does exposure assessments on the basis of either adult data, child data or both (see section 2.2.3). If '3' is entered, the adult-based analysis is performed first.

The analysis continues without further inputs by the user other than continuation returns. COMP3 presents an assessment report for the surface and near-surface soil medium in a format different than that for the other media. Figure 21 is the assessment for the sample problem (Section 5.5), adult-based analysis. The non-chemical and chemical-related data are from DEFAULT.LDS and DEFCHEM.DAT. After a listing of scenario pathways, the display indicates:

ANALYSIS FOR ADULTS: INTAKE CRITERION IS = <adult value> mg/day

When response '2' is selected, the display is:

ANALYSIS FOR CHILDREN: INTAKE CRITERION IS = <child value> mg/day

The intake criterion value is the product  $PHLD \times BW$  discussed in Section 2.1.

The Assessment Computations Table follows. Each "path number" corresponds to the assignments in Table 4. The "pathcode" is that discussed in Section 8.1 for subsite assignments (for applicable routes) and meat/dairy path options. The "unit intake" is the  $TAKE_j(avt)$  described in Section 2.2.3. For example, pathway 11 alone would provide 0.0124 mg/day of pollutant if the subsite #1 topsoil pollutant concentration were 1 mg/kg. The "medium concentration at limit intake" indicates the pollutant concentration in soil that would provide the intake criterion by each pathway\* alone (in this section, "pathway" indicates either a pathway or route). For example, pathway 11 alone would provide 0.1634... mg/day of pollutant (the adult intake criterion) if the subsite #1 topsoil pollutant concentration were 13.15 mg/kg.

A continuation return prompt is then requested, after which the "Assessment by Soil Location" Table is displayed. The table provides results for up to four different soil types, based on the subsite options and pathways selected. For each soil type, two numerical values appear. The leftmost is the hazard index for 1 mg/kg pollutant in the soil type. For example, for subsite #1 topsoil with 1 mg/kg pollutant, the hazard index would be 0.0784. For a baseline assessment, this value can be multiplied by the type soil representative concentration to determine a hazard index for the pollutant and soil type. The sum of products: hazard index per mg/kg  $\times$  representative concentration is the hazard index for the pollutant and scenario. The "soil limit" is similar in meaning to the "medium concentration at limit intake" above, here, the delimiter is soil type rather than pathway. For example, subsite #1 topsoil is involved with pathways 8 and 11, and via these pathways, 12.76 mg/kg pollutant concentration in soil would provide the adult limit, or would correspond to unit hazard. In terms used in Section 2.1,  $SUMTAKE$  is approximately 0.0128, the sum of unit intakes for these pathways. The adult intake criterion (0.1634452 mg/day) divided by  $SUMTAKE$  equals 12.76 mg/kg. Pathway 11 is the more important of these two pathways; the unit intake for pathway 11 is about 30 times that for pathway 8.

After another continuation return, COMP3 displays a correspondence list between the pathways and the soil types.

The "Assessment Computations" Table for the other media is simpler, since there are no sub-divisions within a medium. Figure 22 is an example for a hypothetical water scenario. The "path number" and "pathcode" columns have the same significance discussed above. Three columns of calculated values

```

***** ASSESSMENT BASIS (ADULT OR CHILD) SELECTION *****
Input '1' for adult-based analysis
Input '2' for child-based analysis
Input '3' to do both analyses:: 1
Press ENTER(return) key to continue...
Scenario **. Sample problem for manual
Environmental Medium **. Surface and near-surface soil pathways
Non-chemical data file title **
Default file for starting new .LDS file. Check user's guide for parameter value
derivation.
Scenario pathways **
PATHWAY 8 consume contaminated vegs. grown at #1 subsite
PATHWAY 9 consume beef, livestock grazes on forage grown at #2 subsite
Allowance is made for livestock ingestion of soil and for livestock watering
on surface supply which gets cont. runoff from sub-site.
PATHWAY 11 exposure to dirt at residence (oral, dermal, respired)
PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.
Exposure assumed to be primarily caused by inhalation of vapors in basement.
*****
Press ENTER(return) key to continue...
ANALYSIS FOR ADULTS: INTAKE CRITERION IS... .1634452 mg/day

***** ASSESSMENT COMPUTATION IN SOIL(S) *****
SUBSTANCE NAME IS
2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
PATH NUMBER      PATHCODE      UNIT INTAKE      MEDIUM CONC
                  see manual    mg/day per      AT LIMIT INTAKE
                  mg/kg
# 8               12           3.83E-04        4.273E+02
# 9               19           2.04E-05        7.992E+03
# 11              26           1.24E-02        1.315E+01
# 13              29           1.90E-04        8.602E+02
Press ENTER(return) key to continue...
ASSESSMENT BY SOIL LOCATION

Soil Type          Hazard Index      Public Health
                  per mg/kg        Soil limit, mg/kg*
Subsite #1 Topsoil 7.84E-02         1.276E+01
Subsite #2 Topsoil 1.25E-04         7.992E+03
Basement subsoil   1.16E-03         8.602E+02
-----
* Soil Limit is conc. at which soil pathways provide intake criterion
of .1634452 mg/day.

Press ENTER(return) key to continue...
Soil identification by pathway...
Path 8 -- Subsite #1 Topsoil
Path 9 -- Subsite #2 Topsoil
Path 11 -- Subsite #1 Topsoil
Path 13 -- Basement subsoil
Press ENTER(return) key to continue...

```

Figure 21. COMP3 Assessment of Sample Problem

```

PATHWAY 1 ingest water with pollutant from domestic supply
PATHWAY 7 consume fish from contaminated water
*****
Press ENTER(return) key to continue...
ANALYSIS FOR ADULTS: INTAKE CRITERION IS... .1634452 mg/day

***** ASSESSMENT COMPUTATIONS *****
SUBSTANCE NAME IS
2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...
PATH  PATH-  UNIT INTAKE  MEDIUM CONC  LIMIT INTAKE
NUMBER CODE   mg/day per  AT LIMIT INTAKE  mg/day at Limit Conc.
                  mg/L
# 1     1     1.31E+00    1.24E-01      8.82E-02
# 7     7     1.12E+00    1.46E-01      7.52E-02

PPLV* IS 6.72E-02 mg/L
Hazard index per unit concentration is 14.89024
PUBLIC HEALTH LIMIT INTAKE (reference dose x body weight) is .1634452 mg/day
* PPLV is medium conc for which intake is ADI.
Press ENTER(return) key to continue...

```

Figure 22. COMP3 Assessment for Hypothetical Water Medium-Based Problem

appear. The "unit intake" column indicates, for each pathway, the intake for a 1 mg/L pollutant level in water (or for sediment, 1 mg/kg). The second column, "Medium conc at limit intake" is the pollutant concentration in water (or sediment) for each route, which, in the absence of all others, provides the intake criterion. The "Limit Intake" column is the pro ration of the intake criterion amongst the pathways if the water or sediment pollutant concentration equaled the PPLV. The PPLV and the hazard index per unit concentration follow the tabular entries.

## 9.2 The Constraint Analyses Programs CONWS AND CONTS

After the Assessment Computation of COMP3 (Figure 21 or 22) is concluded, there is a continuation return. Then, either CONTS (for surface and near-surface soil) or CONWS (for water or sediment) is accessed. The initial display in either program briefly explains the two types of constraints, and prompts for an integer input of 0, 1, 2, or 3. The input '0' bypasses the constraint analyses, and this closeout display appears:

```
Ready to return to OPEN3
Hit enter (return) to continue...
```

Alternately, the input '1' at this prompt starts the Type 1 constraint analysis; the input '2', the Type 2 constraint analysis. The input '3' specifies both analyses are to be performed, starting with the Type 1 constraint analysis.

In CONTS, if one assessment analysis was specified in COMP3, the constraint analysis is performed on that basis, and a message is displayed

```
Constraint analysis based on <child or adult> limit
```

If both the adult-based and child-based assessment analyses were performed in COMP3, this prompt appears:

```
Enter '1' to use adult limit in analyses, '2' for child limit:
```

In CONWS, if only one assessment analysis was specified in COMP3, the message shown for CONTS is displayed. If both analyses were specified in COMP3, this prompt is displayed:

```
Adult limit = <Adult PPLV> Child limit = <Child PPLV>
```

```
Select criterion for constraint analysis
```

```
Enter '1' to use adult limit in analyses, '2' for child limit::
```

After the response of '1' or '2', only continuation returns are required. At the conclusion of either CONTS or CONWS, the OPEN3 Main Selection Menu is accessed.

### Type 1 Constraint

**CAUTION:** Constraints are computed based on available online .DAT file data, and in the case of the soil medium analysis, the soil profiles in the scenario. The comparisons displayed may include some that are not of interest. The user will have to resolve the importance and relevance of these to the instant problem.

This analysis operates on candidate constraint factors, determines the corresponding environmental medium concentration at which this factor would be attained (critical concentration), and compares that concentration to the

public health limit. If the critical concentration is less than the "Public Health Soil Limit" (see Figure 2), a potential Type 1 constraint is declared.

Figure 23 is part of the Type 1 constraint analysis for the sample problem, and typifies the displays from CONTS. Note that the first constraint TOL (index 241) is presented for two soil profiles. This illustrates the cautionary statement above; although drinking water intake is not a pathway in the sample problem scenario, an organoleptic limit (TOL) is available, and both subsite #1 and #2 are involved in the scenario. The "Public Health Soil Limits" are the same as in Figure 21. Similarly, since a cattle toxicity limit (CTAEL) is available, the Type 1 constraint analysis for all related pathway/route combinations appears. However, while meat from livestock is an intake pathway, milk from dairy cows is not.

Enter your selection here:: 1

Constraint analysis based on adult limit

\*\*\*\*\* TYPE 1 CONSTRAINT ANALYSIS \*\*\*\*\*

CONSTRAINT 241 TOL, Organoleptic limit - taste in water, mg/L  
Baseline value .01

Soil type Code/Option *****	Public Health Soil Limit (mg/kg)	Critical Conc. (mg/kg)	Potential Type 1 Constraint
Subsite #1 Topsoil	1.28E+01	1.77E+01	No
Subsite #2 Topsoil	7.99E+03	1.11E+02	Yes

Press ENTER(return) to continue...

\*\*\*\*\* TYPE 1 CONSTRAINT ANALYSIS \*\*\*\*\*

CONSTRAINT 243 AQTL, Aquatic toxicity limit in water, mg/L  
Baseline value .05

Soil type Code/Option *****	Public Health Soil Limit (mg/kg)	Critical Conc. (mg/kg)	Potential Type 1 Constraint
Subsite #1 Topsoil	1.28E+01	8.83E+01	No
Subsite #2 Topsoil	7.99E+03	5.56E+02	Yes

Press ENTER(return) to continue...

\*\*\*\*\* TYPE 1 CONSTRAINT ANALYSIS \*\*\*\*\*

CONSTRAINT 247 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day  
Baseline value .01

Soil type Code/Option *****	Public Health Soil Limit (mg/kg)	Critical Conc. (mg/kg)	Potential Type 1 Constraint
***** Livestock for meat *****			
Subsite #1 Topsoil P	1.28E+01	5.07E-01	Yes
Subsite #1 Topsoil PS	1.28E+01	4.73E-01	Yes
Subsite #1 Topsoil PSW	1.28E+01	4.72E-01	Yes

\*\*\*\*\* Dairy animal \*\*\*\*\*

Subsite #1 Topsoil P	1.28E+01	4.19E-01	Yes
Subsite #1 Topsoil PS	1.28E+01	3.92E-01	Yes
Subsite #1 Topsoil PSW	1.28E+01	3.90E-01	Yes

\*\*\*\*\* Livestock for meat \*\*\*\*\*

Subsite #2 Topsoil P	7.99E+03	2.54E-01	Yes
Subsite #2 Topsoil PS	7.99E+03	2.46E-01	Yes
Subsite #2 Topsoil PSW	7.99E+03	2.46E-01	Yes

\*\*\*\*\* Dairy animal \*\*\*\*\*

Subsite #2 Topsoil P	7.99E+03	2.10E-01	Yes
Subsite #2 Topsoil PS	7.99E+03	2.03E-01	Yes
Subsite #2 Topsoil PSW	7.99E+03	2.03E-01	Yes

Press ENTER(return) to continue...

Figure 23. Part of the Type 1 Constraint Analysis for Sample Problem

Figure 24 is the Type 1 constraint analysis for the assessment shown in Figure 22 and illustrates the CONWS display. The format of entries is:

```

***** PPLV = <computed value, units> vs.
Critical conc. = <computed value, units> based on CONSTRAINT
<Constraint dataname> = <online value from .DAT file>
POTENTIAL TYPE 1 CONSTRAINT or NO TYPE 1 CONSTRAINT

```

The analysis concludes with the message: "End Type 1 Constraint Analyses" which is followed by either a closeout display when only the Type 1 analysis is selected or by the Type 2 Constraint header:

```

***** TYPE 2 CONSTRAINT ANALYSIS FOR <medium>

```

A portion of the Type 2 constraint analysis in CONTS is shown in Figure 25. The comparison is on a pathway by pathway basis, between the water concentration back-calculated from the soil profile limit and the pollutant's aqueous solubility limit. The narrative format is:

---

```

***** TYPE 1 CONSTRAINT ANALYSIS *****
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = .01 mg/L based on CONSTRAINT
241 TOL, Organoleptic limit - taste in water, mg/L = .01
POTENTIAL TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = .05 mg/L based on CONSTRAINT
243 AQTL, Aquatic toxicity limit in water, mg/L = .05
POTENTIAL TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = 5 mg/L based on CONSTRAINT
244 PHLW, Phytotoxicity limit in water, mg/L = 5
NO TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = 1.333333 mg/L based on CONSTRAINT
245 PHLS, Phytotoxicity limit in soil, mg/kg adjusted to water medium basis. =
20
NO TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
Case 1 -- Steers/Water Intake Only
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = .1633987 mg/L based on CONSTRAINT
247 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day = .01
NO TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
Case 2 -- Steers/Water and Plant Intake
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = 2.187227E-02 mg/L based on CONSTRAINT
247 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day = .01
POTENTIAL TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
Case 1 -- Dairy Cows/Water Intake Only
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = 6.666666E-02 mg/L based on CONSTRAINT
247 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day = .01
POTENTIAL TYPE 1 CONSTRAINT
Press ENTER(return) to continue...
Case 2 -- Dairy Cows/Water and Plant Intake
***** PPLV = 6.715809E-02 mg/L vs.
Critical conc. = 1.590214E-02 mg/L based on CONSTRAINT
247 CTAEL, Cattle toxicity adverse effects limit, mg/kg-day = .01
POTENTIAL TYPE 1 CONSTRAINT
Press ENTER(return) to continue...

```

Figure 24. Type 1 Constraint Analysis, Problem from Figure 22



PATHWAY <number, followed by description>  
Water conc. corresponding to soil limit is <value>  
Soil <profile identification> limit is:: <soil limit in mg/kg>  
Type 2 constraint (detected)(not detected) for pathway

The Type 2 constraint analyses in CONWS is less complex. For water as the environmental medium, the PPLV is compared to solubility. If the PPLV exceeds solubility, this message appears:

Type 2 constraint exists. Public health limit conc.  
may not be relevant for this analysis since  
Wsol, Water solubility, mg/L = <value of Wsol> is less than limit.

If solubility exceeds the PPLV, only this message appears:

Public health conc. limit not subject to Type 2 constraint.

When sediment is the environmental medium, a water concentration corresponding to the sediment PPLV is back-calculated, and the back-calculated value is displayed prior to the above messages.

---

Press ENTER(return) to continue...  
End Type 1 Constraint Analysis  
\*\*\*\*\* TYPE 2 CONSTRAINT ANALYSIS FOR  
Surface and near-surface soil pathways  
Substance is::  
2,4,6-Trinitrosomething, CAS 1234-56-7, Default name for something...

Most analyses based on criterion that water conc. corresponding to a Public Health Soil Limit exceeds solubility limit of .001 mg/L. After each test, enter a return continuation.  
PATHWAY 8 consume contaminated vegs. grown at #1 subsite  
Water conc. corresponding to soil limit is .6358161 mg/L  
Soil Subsite #1 Topsoil - limit is:: 12.76174  
Type 2 constraint detected for pathway.

Press ENTER(return) to continue...  
PATHWAY 9 consume beef, livestock grazes on forage grown at #2 subsite  
Allowance is made for livestock ingestion of soil and for livestock watering on surface supply which gets cont. runoff from sub-site.  
Water conc. corresponding to soil limit is 793.5793 mg/L  
Soil Subsite #2 Topsoil - limit is:: 7992.478  
Type 2 constraint detected for pathway.

Press ENTER(return) to continue...  
PATHWAY 11 exposure to dirt at residence (oral, dermal, respired)  
Water conc. corresponding to soil limit is .6358161 mg/L  
Soil Subsite #1 Topsoil - limit is:: 12.76174  
Type 2 constraint detected for pathway.

Press ENTER(return) to continue...  
PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.  
Exposure assumed to be primarily caused by inhalation of vapors in basement.  
Water conc. corresponding to soil limit is 412.8808 mg/L  
Soil Basement subsoil - limit is:: 860.1682  
Type 2 constraint detected for pathway.

Press ENTER(return) to continue...  
Ready to return to OPEN3  
Press ENTER(return) to continue...

Figure 25. Type 2 Constraint Analysis, Sample Problem

## 10.0 CHEMICAL-RELATED DATA ESTIMATION SUBROUTINES

CRDES3 and its two satellite programs CRD013 and CRD113 provide information and methods to estimate chemical-related data. Estimation methods that require chemical-related inputs only are in CRD013, and are discussed in detail in Section 10.3. Estimation methods that require both chemical-related and non-chemical data inputs are in CRD113, which is discussed in Section 11.

The estimation methods incorporated in CRD013 and CRD113 were selected for wide applicability, minimal input requirements, and ability to be executed without extensive coding. They are not necessarily the most accurate estimation methods available. Many methods have been adapted from Lyman et al.<sup>9</sup>; and that reference provides many other methods and additional background information.

### 10.1 General CRDES3 Access and Exit Procedures

CRDES3 is entered from OPEN3 by responding '9' to the OPEN3 Main Selection Menu Prompt. CRDES3 is entered from CHMF3 by either user direction (see Section 7.4) or under DUST control (see Section 7.2). For convenience of discussion, these are called entry modes 1, 2, and 3 respectively. When entry modes 1 and 2 are used, the CRDES3 Selection Menu (see Figure 13) is displayed. The user enters an integer in response to the menu's "Input the subroutine number: " prompt to access a specific subroutine. With entry mode 3, this menu does not appear. Rather, the subroutine corresponding to the current dataname index displayed in CHMF3 is directly entered.

Some subroutines provide only descriptive messages\*. The messages provide the information that would be printed out in PTLL3 or stored in PTL3D. After any subroutine is accessed, the following prompt appears:

```
** CRDES Central Processor: Wish to do more in CRDES3?  
Enter 'yes' or 'no'::
```

The CRDES3 processing of a 'yes' or 'no' input depends upon the entry mode to CRDES3. The various combinations are tabulated below:

Entry Mode	Respond 'yes'	Respond 'no'
1	Return to the CRDES3 Selection Menu	Return to the OPEN3 Main Selection Menu.
2	Re-enter the subroutine just performed.	Return to the CHMF3 Main Selection Menu
3	Re-enter the subroutine just performed.	Return to the data review and change routine prompt in CHMF3

\* For entry modes 1 and 2, a response of '1', '2' or '3' to the CRDES3 Selection Menu prompt ( DTol & DTos, DTil & DTis, DTdl & DTds) will generate two separate description messages, one each for the adult- and child-related datanames.

## 10.2 Estimation Method Subroutines Procedures

These subroutines start with a description message display, followed by a method selection prompt. Based on message length, a continuation return may be needed to proceed from the message to the method selection prompt. The user selects a method by input of a specified integer. The user can exit the subroutine with a prompt of '0'. In that case, the "CRDES Central Processor" prompt discussed above appears.

When an estimation method is selected, input data are collected. If CRDES3 is accessed from OPEN3, all chemical-related data are provided by the user as prompted. If CRDES3 is entered from CHMF3, the required data are retrieved from the online chemical-related database without any prompts. After an estimation method is completed, all input data to the estimation equations are displayed. The estimation result appears in the following format:

```
<index number dataname> = <estimate>
Estimate by method # <number from method selection menu>
```

If CRDES3 was accessed from OPEN3, the CRDES Central Processor prompt follows. Otherwise, the display continues with the following message and prompt:

```
CHMF3 Online value is: <current value>
Replace online value with estimate? (yes/no):
```

The dataname value currently in CHMF3 remains online unless the user enters a 'yes' response here to replace it. After the 'yes' or 'no' response, the CRDES3 Central Processor prompt occurs.

## 10.3 Estimation Subroutines in CRD013

### 10.3.1 Water Solubility (Wsol)

Four equations options are available. The equations are octanol-water partition coefficient-based correlations, and have been presented in Lyman et al.<sup>9</sup>. Equations 2.2 and 2.15 from Lyman et al.<sup>9</sup> compute a molar water solubility, and molecular weight data is required to convert to a mg/L basis. Equation 2.15 is presented in two formats; one includes a melting point correction term. This additional term is claimed to be somewhat more accurate for substances that are crystalline solids above 25 °C<sup>9</sup>. If this option is selected, the melting point in °C is requested. If the melting point is below 25 °C, the input is ignored in calculations.

### 10.3.2 Boiling Point (Tb)

Two methods are presented. Method '1' is an inverse form of the Lorenz and Herz correlation<sup>10</sup> which predicts the melting point from the boiling point. The equation used is:  $T_b = 1.713T_m$ , where  $T_b$  and  $T_m$  are the boiling and melting point temperatures in degrees Kelvin. It is not recommended for aldehydes, alcohols, and polar hydrocarbons.

Method '2', developed by Miller, is discussed in Section 12-5 of Lyman et al.<sup>9</sup>. The user must know the pollutant's molecular structure to apply this method. Figure 26 shows the information message for the method followed by

the presentation tableau indicating the applicable fragment and structures. After the message and tableau, this prompt appears:

Enter 'yes' or 'no'  
Do you wish to continue analysis?

If the user responds 'no', the subroutine is terminated. If the user responds 'yes', the presentation tableau is displayed. This tableau follows the order of Table 12-12 in Lyman et al.<sup>9</sup>. The subroutine prompts for a fragment identifier number (FIN) input followed by the number of times an identified fragment occurs in the pollutant molecule. After their input, the tableau display is updated to reflect the last input, and this message is displayed:

Enter 'yes' or 'no'  
Do you want to do more?

If the response is 'yes', a FIN and the number of FIN fragments is again requested. For example, in Figure 26, the user is about to substitute 2 of 3 positions on a propane substrate with bromine. The user provides paired entries until all structure fragments have been entered. The user can correct errors, or replace a non-zero value with zero. After all entries have been made, respond 'no' to the above message to proceed.

\*\*\*\*\* BOILING POINT ESTIMATION MENU \*\*\*\*\*

Select '0' to exit without calculation  
Select '1' to do 'rough approximation' estimate  
Select '2' to do Miller's method. Enter selection:: 2

The CRT will display 41 different structure fragments in a table. You will be prompted to enter the identification number for a given fragment (FIN) of the subject pollutant and then the number of times that fragment occurs in the pollutant molecule. Your entry will be echoed back. You will be queried if you wish to do more. If you select yes, the table will re-display with the previous selection posted. This sequence is repeated until you respond 'no' to the 'Do you want to do more?' query.

In the table, there are coded abbreviations. 'NR' indicates a non-ring structure, 'RG' a ring. Rings can be either aliphatic or aromatic. Other abbreviations are alc=alcohol, phl=phenol, ald=aldehyde, est=ester. A triple bond is shown as '='. As examples of input, dinitrophenol would appear as 3FIN14 (=CH- in a ring), 3FIN15 (=C< in a ring), 1FIN22 (phenolic OH), and 2FIN37 (nitro groups). 1,2-dibromo-3-chloropropane or CH2Br-CHBr-CH2Cl appear as 2FIN2 (-CH2- non-ring), 1FIN3 (-CH< non-ring), 2FIN19 (bromine), and 1FIN18 (chlorine). FIN order of entry is not required.

Enter 'yes' or 'no'.  
Do you wish to continue analysis?: yes

MILLER BOILING POINT METHOD FRAGMENTS ID TABLE			
OFIN1 -CH3 [NR]	2FIN2 -CH2-[NR]	1FIN3 -CH< [NR]	OFIN4 >C< [NR]
OFIN5 =CH2 [NR]	OFIN6 =CH- [NR]	OFIN7 =C< [NR]	OFIN8 =C= [NR]
OFIN9 ==CH [NR]	OFIN10 ==C- [NR]	OFIN11 -CH2- [RG]	OFIN12 -CH< [RG]
OFIN13 >C< [RG]	OFIN14 =CH- [RG]	OFIN15 =C< [RG]	OFIN16 =C= [RG]
OFIN17 -F	OFIN18 -Cl	OFIN19 -Br	OFIN20 -I
OFIN21 -OH alc	OFIN22 -OH phl	OFIN23 -O- [NR]	OFIN24 -O- [RG]
OFIN25 >C=O [NG]	OFIN26 >C=O [RG]	OFIN27 -CH=O ald	OFIN28 -COOH acid
OFIN29 -COO- est	OFIN30 =O other	OFIN31 -NH2	OFIN32 >NH [NR]
OFIN33 >NH [RG]	OFIN34 >N- [NR]	OFIN35 >N- [RG]	OFIN36 -CN
OFIN37 -NO2	OFIN38 -SH	OFIN39 -S- [NR]	OFIN40 -S- [RG]
OFIN41 =S			

When prompted, enter FIN. Enter number of units next  
Enter FIN (from 1 to 41) here:: 19

Enter number of specified fragments in molecule. 2

Figure 26. Miller's Boiling Point Method Displays

The molecular weight used in Miller's method is computed from fragment inputs. If CRDES3 was accessed from CHMF3, the online molecular weight is also displayed. If these weights differ other than due to round-off (fragment weights are computed to the nearest 0.1 unit), the user should check for either an incorrect input for pollutant structure or an incorrect online molecular weight.

### 10.3.3 Vapor Pressure (VP)

Five methods are provided for vapor pressure, each is summarized in the information message (Figure 27). After the method prompt response, the temperature for vapor pressure calculation is requested by the prompt:

"Enter temperature in DegC for calculation result:"

Any vapor pressure inputs required in the methods discussed below must be in mm Hg (torr) units.

Mackay's method #1. The algorithm used is presented in Mallon, et al<sup>11</sup>:

$$\ln VP = -(4.4 + \ln Tb) \times (1.803 [Tbr-1] - 0.803 \ln[Tbr]) - 6.8(Tmr-1)$$

where Tb is the boiling point, Tbr is the boiling point relative to the calculation temperature (Tcalc), or Tb/Tcalc, and Tmr, the relative melting point, or Tm/Tcalc. In this algorithm, temperatures are in degrees Kelvin, and the calculated VP is in atmospheres. If CRDES3 is accessed from OPEN3, the user supplies the melting point and boiling point temperatures in °C.

Watson's boiling point method. This is described in Lyman et al.<sup>9</sup>, sections 14-3 and 14-4. If CRDES3 was accessed from OPEN3, the user supplies the substance's boiling point in °C. Then, the user is prompted:

"Is substance a liquid at calculation temp?"

For a substance in the liquid state, the response is 'yes'; 'no' for the solid state. This sequence appears in Figure 28.

Next, the Watson Method Index Table is displayed; see Figure 28. This table identifies classes of compounds, and the user enters the index number corresponding to the classification that best describes the substance (in Figure 28, '19' has been entered, the index for a "nitro compound"). A default (index number 35) is also provided. The index number identifies a K<sub>F</sub> value (KFCAL), which is required to calculate the key equation 14-16 of Lyman et al.<sup>9</sup>. KFCAL data are in Table 14-4 of Lyman et al.<sup>9</sup>, and in the estimation method, the six-carbon entries are used.

If CRDES3 is accessed from CHMF3, the online stored boiling point and melting point temperatures determine whether a substance is liquid or solid at the calculation temperature. In this case, the first prompt for method input is the query for index number: "Enter identification number:"

Linear method. This method is based on the Clausius-Clapeyron equation:  $\log P = K1 + K2/T$ , where K1 and K2 are constants and T is in absolute temperature units. The program prompts for paired temperature and pressure data, first for the lower end of the range, and next for the upper end of the range. The program checks for correct order, and repeats the prompt if the sequence of inputs was incorrect.

\*\*\*\*\* INFORMATION ON \*\*\*\*\*

191 VP, Saturated vapor pressure, mm Hg

The saturated vapor pressure (VP) is exerted by a substance when it is placed in a closed container and allowed to equilibrate. Here, VP is in mm Hg units. VP is temperature-related. VP is used to estimate the Henry's Law Constant used in volatility pathways from soil and water.

PHAS3 has 5 methods to estimate VP. The methods are discussed in detail in Section 10.3.3 of the User's Manual. The 5 methods are: Mackay's # 1 (melting\* and boiling point\*); Watson's boiling point (boiling point\* and molecular structure details\*\*); simple interpolation (paired temperature and vapor pressure data\*\*); Mackay's modified (melting point\*); and Watson's reduced pressure (paired temperature and reduced boiling point and molecular structure details\*\*). \* - User input if access from OPEN3; \*\* - User input, all access modes. If access if from OPEN3, you should know the substance phase state at calc. temperature, and, if you provide vapor pressure data at a different temperature, you must know the substance's phase state at that temperature. VPs of better known pollutants at ambient temperature have been compiled; see SPHEM (OSWER 9285.4-1, EPA540/1-88-060) or Callahan et al., EPA440/4-79-029 (129 Priority Pollutants) or the Documentation of the TLV (ACGIH, 5th Edition). Several computer-accessible databases include VP data for listed substances. Press ENTER(return) key to continue...

Figure 27. Vapor Pressure Routine Information Message

Enter your selection (from 0 to 5):: 2  
Enter temperature in DegC for calculation result:: 25  
Enter boiling point temp. in degC:: 130  
Enter 'yes' or 'no'.  
Is substance a liquid at calculation temp?:: no  
You will be shown a table of general compound groups. Choose the number of the group describing your compound. Note, for mixed aromatic constituents, -OH takes precedence. For simple aromatics consider the phenyl group as a n-Alkane (selection #1).  
Press ENTER(return) key to continue...

\*\*\*\*\* WATSON METHOD INDEX TABLE FOR VAPOR PRESSURE ESTIMATIONS \*\*\*\*\*

\*\*\* Aliphatic or Carbocyclic/ Heterocyclic Cmps. with Aliphatic Properties

- |  |                                     |                     |
|--|-------------------------------------|---------------------|
| 1. n-Alkanes   | 2. Other alkanes                    | 3. Olefins          |
| 4. Cyclic sat. hydrocarbs  | 5. Alkylated cyclic sat. hydrocarbs |                     |
| 6. Monochloride  | 7. Monobromide                      | 8. Monoiodide       |
| 9. Polyhalide (not entirely halogenated)                             | 10. Totally halogenated cpd.        |                     |
| 11. Perfluorocarbon  | 12. Ester (R-COO-R')                | 13. Ketone          |
| 14. Aldehyde   | 15. Primary amine                   | 16. Secondary amine |
| 17. Tertiary amine   | 18. Nitrile                         | 19. Nitro compound  |
| 20. Mercaptans   | 21. Sulfides                        |                     |
| 22. Alcohol(single OH)   | 23. Diols                           | 24. Triols          |
| 25. Cyclohexanol, cyclohexyl methyl alcohol, etc.                    |                                     |                     |
| 26. Aliphatic ethers   | 27. Oxides (cyclic ethers)          |                     |
| *** Aromatic Compounds (use phenol values if mixed function on ring) |                                     |                     |
| 27. Monophenols  | 28. Other phenols(2 or more -OH)    |                     |
| 29. Monoaniline  | 30. Other aniline(2 or more -NH2)   |                     |
| 31. N-sub. anilines (C6H5NHR)  | 32. Naphthols (one -OH)             |                     |
| 33. Naphthylamines (one -NH2)  | 34. N-Substitued naphthylamines     |                     |
| 35. ANY OTHER COMPOUND(Default value)                                |                                     |                     |

Enter identification number:: 19

KFCAL= 1.05

Boiling Point (C) = 130

Ambient state of substance is solid

VP computed at 25 degC.

191 VP, Saturated vapor pressure, mm Hg = 7.828869

Estimate by method # 2

\*\* CRDES3 Central Processor: Wish to do more ir CRDES3?

Enter 'yes' or 'no'::

Figure 28. Watson's Vapor Pressure Method Display. CRDES3 access from OPEN3.

When CRDES3 is accessed from OPEN3, the next query is:

PHASE STATUS: For state of substance in range and at calc. temp  
Enter '1' if substance is a LIQUID in range and LIQUID at calc. temp  
Enter '2' if substance is a SOLID in range and SOLID at calc. temp  
Enter '3' if substance is a LIQUID in range BUT a SOLID at calc. temp

The user enters the applicable integer. If the response is '3', the user is then prompted to supply the pollutant's melting point in °C. The program then checks for consistent temperatures in a sequential manner; there are four outcomes\*:

Melting point > upper end range temperature: the calculation proceeds and this message is issued: "Solid state at <calc. temp> temp. and in range"

Melting point > lower end temperature but < the higher end temperature. This message is issued: "Solid-liquid change in range, can't do estimate. Please recheck inputs." and the program backs-up to the prompt for paired temperatures and pressures.

Melting point > Tcalc, but < the temperature range: the calculation proceeds and this message is issued: "Solid state at <calc. temp> temp. and liquid in range"

Melting point > Tcalc and > temperature range: the calculation proceeds and this message is issued: "Liquid at <calc. temp> temp. and in range."

If CRDES3 is entered from CHMF3, the database values of melting point, boiling point, and range inputs are automatically checked against Tcalc according to the above sequence. This process is announced by the message:

"Determining phase status for estimate...."

If there is no phase transition between the Tcalc and the temperature range, a linear equation is computed to calculate vapor pressure at Tcalc. If a transition exists, the linear equation computes (but does not display) the vapor pressure of the substance as a "supercooled liquid". The corresponding solid vapor pressure is then computed by equation 14-10 of Lyman et al.<sup>9</sup>.

This method is most accurate when Tcalc is inside the range. In case of an extrapolation of more than about 25 °C outside of the range, Watson's reduced pressure method (see below) may be more accurate; moreover it only requires one data set.

Mackay's method (modified). This method uses the Lorenz and Herz equation (see Section 10.3.2) to estimate the boiling point. Then, the melting point and estimated boiling point are entered into Mackay's Method #1. The user enters the melting point when CRDES3 is accessed from OPEN3. When CRDES3 is accessed from CHMF3, a boiling point is computed from the online melting point, and is displayed. However, that computed boiling point does NOT replace the online boiling point.

\* This is not all inclusive. From a practical point, Tcalc is either lower than or within the known vapor pressure-temperature range. The sequential check covers practical combinations of Tcalc, melting point, and temperature range for input vapor pressure data.

Watson's reduced pressure method. This routine is based on equations 14-24 and 14-26 in Lyman et al.<sup>9</sup>. In place of the boiling point (the temperature corresponding to a 1 atmosphere vapor pressure), a set of paired vapor pressure-temperature data are entered. Usually, the vapor pressure entry is sub-atmospheric, hence the term "reduced pressure". The user provides the reference temperature and pressure at the two prompts:

Enter reference temperature for reduced pressure:

Enter VP at reference temperature:

If CRDES3 is accessed from OPEN3, this additional query appears:

"Is substance a liquid at calculation state?"

Respond 'yes' for liquid or 'no' for solid. Then the Watson Method Index Table (see Figure 28) is displayed. After the index number is entered, the conditions of the problem and estimated vapor pressure are displayed.

#### 10.3.4 Soil Organic Carbon-Water Partition Coefficient (Koc)

This subroutine provides seven different correlation equations. The display screen shown in Figure 29 identifies these equations and the requisite inputs. Figure 29 shows the input prompt for one method with CRDES3 access from OPEN3. Otherwise, only the method selection integer is needed.

#### 10.3.5 Soil to Vegetable and Plant Partition Coefficients (Ksv and Ksp)

Although Ksv and Ksp are separate selections in the CRDES3 Selection Menu, one subroutine processes both. Two methods are available. The first is an equation suggested by Travis and Arms<sup>12</sup> to estimate Ksv.

$$\log K_{sv} = 1.588 - 0.578 \times \log P$$

The second method estimates Ksp as  $10 \times K_{sv}$ . When CRDES3 is accessed from OPEN3, the logP value is requested; otherwise there are no further inputs.

There are some restrictions to this subroutine. If method 2 is attempted while Ksv is the selected datum, the subroutine issues a caution message and reissues the initial Ksv/Ksp Menu display. If method 2 is attempted while Ksp is the selected datum, Ksv is not available to replace the online Ksv as part of the procedure. The Travis and Arms equation method only estimates Ksv explicitly when Ksv is the selected datum.

#### 10.3.6 Plant to Adipose Tissue Partition Coefficient (Kpat)

Two equations are provided, both from Garten and Trebalka<sup>13</sup>:

$$\begin{aligned} K_{pat} &= 10 ( -3.935 + 0.511 \log P ) \\ K_{pat} &= 10 ( -1.633 - 0.608 \log W_{sol} ) \end{aligned}$$

When CRDES3 is entered from OPEN3, logP is requested for the first selected method; water solubility is requested for the other.



192 Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)

Koc is the ratio between the equilibrium pollutant concentration on soil organic carbon (OC) and its concentration in water. Koc can indicate the relative distribution of pollutant between soil and water assuming that pollutant in soil is primarily physically adsorbed on OC. This appears to be a fairly good assumption for non-polar organic substances. However, the source of organic carbon can be a factor, and regression equations to estimate Koc are less accurate than for analogous terms.

Seven methods are presented here. The first six were presented in Lyman and Loreti's (L/L) Final Report for Task 15, EPA Contract 68-01-6951. The Kenaga eqtn. is equation 4-5 in Lyman, et. al. CPEM.

Menu indicates specific equation inputs (LogP, Wsol, MW)

Meth.	Eqtn	Inputs	* Meth.	Eqtn	Inputs
0	Exit w/o Calculation		1	L/L general eqtn.	LogP
2	L/L non-aromatic eqtn.	LogP	3	L/L aromatic eqtn.	LogP
4	L/L general eqtn.	MW, Wsol	5	L/L non-aromatic eqtn.	MW, Wsol
6	L/L aromatic eqtn.	MW, Wsol	7	Kenaga eqtn.	Wsol

Enter your method selection (from 0 to 7):: 2

Enter LogP: 3.26

192 Koc, Organic carbon/water p.c., mg/L per mg/kg (OC) = 1219.158

Estimate by method # 2

Figure 29. Display for Koc Estimation Method 2. CRDES3 Access From OPEN3.

### 10.3.7 Diffusivity in Air (Da)

Two options are presented: an empirical equation and the Fuller, Schettler and Giddings (FSG) method discussed in Section 17-4 of Lyman et al.<sup>9</sup>. After the user selects either method, the computation temperature (°C) is requested.

The empirical equation was suggested by Small<sup>14</sup>

$$Da = 8 ( T_{calc} / 298.2 )^{1.75} / (MW)^{0.5}$$

where Da is in m<sup>2</sup>/day, and Tcalc is in degrees Kelvin. A molecular weight input is required (along with Tcalc) to evaluate Da.

The FSG method computes a "LeBas Volume" as an intermediate result. This volume is estimated from factors based upon a pollutant's empirical formula and structure. These factors appear in Table 17-5 of Lyman et al.<sup>9</sup> The instructions for LeBas Volume estimation are shown in Figure 30, as are the atoms/structures of Table 17-5. At the prompt: "Enter ID# of constituent here: " the user furnishes the atom/structure constituent index number. Then the cursor moves to the right of the indexed item in the tableau; here the user enters the number of times the given item appears in the molecule. After an entry, this prompt appears near the bottom of the screen:

Do you want to do more (yes or no) ?

When the user responds 'yes', the routine to enter information continues. In Figure 30, the instruction example is being followed, and entries have been made for carbon, hydrogen, and two carboxylic oxygen atoms. The user intends to add more information to the tableau.

When the user responds 'no' to the prompt, the Da computation starts. The subroutine determines and displays the molecular weight from tableau inputs. If CRDES3 is entered from CHMF3, the online molecular weight is also displayed. If these weights differ other than due to round-off (fragment weights are to the nearest 0.1 units), the user should check for either an incorrect input for a structure component or an incorrect online molecular weight.

```

***** INFORMATION ON *****
206 Da, Molecular diffusivity in air, m2/sec
The air diffusivity coefficient (Da) indicates a substance's ability to
diffuse in quiescent air. Da is input to water-intake pathways equations
where the volatility of inhaled substances from contaminated water
is involved. Da is input to soil-based pathways involving the
diffusion of substances from soil-pore air in terms of flux (mg/m2-day).
In soil-based pathways, the air conc. is a function of the soil flux model,
the area contaminated and the model treatment of air transfer over the
contaminated area.
Two methods are available in CRD013 to estimate Da. The first, a rough
approximation, only requires MW. The second method was developed by Fuller,
Schettler and Giddings (FSG), see Section 17.4 of Lyman et al. CPEM.
The FSG method requires MW, and structural inputs and is restricted to
compounds with C,H,O,N,S,P,F,Cl,Br & I elemental constituents.
***** Da ESTIMATION MENU SELECTIONS *****
Select '0' to exit without calculation
Select '1' for rough approximation
Select '2' for FSG method
Enter your selection:: 2
Enter temperature of computation in Deg C:: 22

***** INSTRUCTIONS FOR FSG METHOD WITH LEBAS VOLUME *****
The CRT will display the FSG method structure units in a tableau.
You are prompted to enter the index number for an element or
structural component in the pollutant molecule. The cursor will
move to that item in the tableau. There, you enter the
number of units in the pollutant molecule. For example,
if your molecule was CH2Cl-CHBr-COOH, you would enter:
ID#1 [C] - 3; ID#2 [H] - 4; ID#4 [Br] - 1; ID#6 [Cl],1 ; and
ID#9 [Carboxylic O] - 2. At the end of each entry sequence, you
are prompted to continue with entries. The sequence is repeated
if you respond 'yes' to this prompt.
Pres; ENTER(return) key to continue...

LEBAS VOLUME ELEMENTS/COMPONENT INDEX
ID#1 (C) 3 ID#2 (H) 4
ID#3 (O in Meth esters/ethers) 0 ID#4 (Br) 0
ID#5 (O in Eth ester/ethers) 0 ID#6 (Cl) 0
ID#7 (O in other esters/ethers) 0 ID#8 (F) 0
ID#9 (O in carboxylic acids) 2 ID#10 (I) 0
ID#11 (O bonded to S,P or N) 0 ID#12 (S) 0
ID#13 (other bonded O) 0 ID#14 (3 member ring) 0
ID#15 (Double bonded N) 0 ID#16 (4 member ring) 0
ID#17 (N in primary amines) 0 ID#18 (5 member ring) 0
ID#19 (N in sec. amines) 0 ID#20 (6 member ring) 0
ID#21 (P) 0 ID#22 (Anthracene ring) 0
ID#23 (Naphthalene ring) 0
Enter ID# when prompted. Then cursor will move to ID# location
in the tableau. At that location, enter the number of units.
Enter ID# here::

```

Figure 30. Information Message for Da and LeBas Volume Displays

**CAUTION:** If the LeBas Volume computed is less than 1, structural components are probably missing from the input, and an error message is issued. Then, the program returns to the FSG method instruction message.

### 10.3.8 Diffusivity in Water (Dw)

Two methods are presented. In the first, Dw is approximated as 0.0001 Da. When CRDES3 is entered from OPEN3, the user enters Da when prompted. Otherwise, no additional input is required.

The second method is based on the Hayduk and Laudie equation described in Section 17-7 of Lyman et al.<sup>9</sup>. Calculations are restricted to 20 °C for two reasons: the pathway intake equations that use Dw also use EIW data (index 3 or 28 in Table 3), which is computed for 20 °C, and, at 20 °C, the viscosity-dependent term in the Hayduk and Laudie equation is nearly unity.

The second method requires calculation of the LeBas Volume, and the procedure follows that described in section 10.3.7. After the LeBas Volume is computed, this statement appears: "Going back to Dw subroutine", which is followed by the computed Dw.

#### 10.3.9 Henry's Law Constant (Kh)

Kh is evaluated as the saturation vapor pressure divided by the water solubility, both evaluated at a given temperature, and expressed in dimensionless form. After the initial display, this prompt appears:

Is temperature of calculation 25C (298.2K) ?

If the answer is 'no,' the user is prompted to enter a temperature. When CRDES3 is entered from CHMF3, there are no further inputs, and the result is displayed. When CRDES3 is entered from OPEN3, the user is first queried for molecular weight. Then the user is queried for the units of the water solubility datum to be entered:

Water solubility units for input. Enter '1' for mg/L units,  
'2' for mole/L units, '3' for millimole/L units:

After the user enters the applicable integer, the water solubility data is requested. This sequence is repeated for saturation vapor pressure. The accepted pressure units are torr or mm Hg ('1'), atmospheres ('2'), and pascals ('3').

#### 10.3.10 Dermal Permeability Coefficient (PC)

CRD013 uses the equation presented by Fiserova-Bergerova and Pierce<sup>15</sup>:

$$\text{flux} = \text{Wsol}/15 \times (0.038 + 0.153 P) \times \exp(-0.016 MW)$$

where flux is the transfer of substance in mg/cm<sup>2</sup>-hr, Wsol is in mg/cm<sup>3</sup> and P is the octanol-water partition coefficient. The term flux/Wsol has units of cm/hr, and corresponds to PC.

When CRDES3 is accessed from OPEN3, the user provides, when prompted, the log octanol-water partition coefficient and molecular weight.

#### 10.3.11 Fish Bioconcentration Factor (BCF)

Three estimation options are presented, corresponding to equations 5-2, 5-3 and 5-4 in Table 5-1 of Lyman, et al.<sup>9</sup>. These equations respectively require an input of logP, water solubility, or Koc; if CRDES3 is accessed from OPEN3, the routine prompts for the required input.

#### 10.3.12 Water to Vegetable and Plant Partition Coefficients (Kwv and Kwp)

Kwv and Kwp are handled in one subroutine with four method options. The first two methods involve use of Ksv and Ksp, respectively, to compute Kwv or Kwp, with the internal assumption that the forage partition coefficient is 10 times higher than the vegetable coefficient, as mentioned in Section 10.3.5. For Kwv, these relations can be summarized as the following:

$$Kwv = [ Ksv \text{ or } Ksp/10 ] * foc(\text{experimental}) * Koc$$

If CRDES3 is accessed from OPEN3, the user enters, when prompted, the experimental soil Ksv (or Ksp), the foc(experimental), and the substance Koc.

The third method initially uses the Travis and Arms equation (see Section 10.3.5) to implicitly estimate Ksv, followed by the above equation, with an arbitrary foc(experimental) of 0.015, to estimate Kwv or Kwp. If CRDES3 is accessed from OPEN3, the user provides Koc. As discussed in Section 10.3.5, the Ksv estimate is not available for direct substitution for the online Ksv.

The last method uses the "modified" Briggs equation<sup>16</sup>:

$$K_{wp} = 5 \times (0.82 + 10^{E1}) \times 10^{E2}$$

where  $E1 = 0.95 \log P - 2.05$  and  $E2 = -0.178 (\log P - 1.78)^2$ . The coefficient of 5 replaces 0.784 in the reference version; this change accounts roughly for the difference between dry and wet plant weight.

The user provides logP if CRDES3 is accessed from OPEN3. If this equation is used to estimate Kwv, a default conversion is included that  $K_{wv} = K_{wp}/10$ .

#### 10.3.13 Fish Bioaccumulation Factor (BAF)

Two "methods" are provided to estimate BAF. The first involves BCF and an adjustment factor that is a function of the octanol-water partition coefficient. This is believed to be applicable when the fish consume an appreciable amount of food from sediment, such as carp or catfish. At a given logP, BAF will exceed BCF, accounting for water-sediment partitioning, but the difference is only important when logP is higher than about 4.5.

The second method is to set BCF equal to BAF. This is useful only when CRDES3 is entered from CHMF3. If CRDES3 is entered from OPEN3, selection of this method is followed by the message "Method 2 not applicable for OPEN3 entry".

There is evidence that at logP higher than about 4.5, the BAF would be lower than an estimated BCF because of slower kinetics of transfer of larger molecules into fish. PHAS3 does not account for this effect.

## 11.0 CRD113

CRD113 subroutines require both non-chemical and chemical-related data inputs. Moreover, several subroutines, particularly those which estimate "MK" partition coefficients, require considerable non-chemical data. For all 3 modes of entry, CRD113 accesses all non-chemical data from a .LDS file. There are three accession options: (1) use DEFAULT.LDS, (2) specify the .LDS file to be used, or (3) use online data previously downloaded from a .LDS file. The options are listed in the "Non-Chemical Data Accession Subroutine" section of Figure 31. First, past .LDS operations are summarized, followed by a listing of .LDS files on the Disk 2 device. Then the three accession options are presented. In Figure 31, accession option '2' has been selected, and the file DOWNLOAD.LDS selected for downloading. If the option to exit ('0') were selected, the CRDES Central Processor prompt would next appear.

After non-chemical data accession, non-chemical data inputs to a selected estimation method are checked for zero values. If any occur, a message is issued with the format:

```
Missing non-chemical data for <specified non-chemical dataname>
Leaving estimation routine for <dataname associated with subroutine>
```

and the user is sent to to the CRDES Central Processor prompt.

If CRDES3 is accessed from OPEN3, chemical-related data are supplied by the user. Otherwise, CRD113 checks online chemical-related data that are inputs to the selected estimation method for zero values. If any datum with a zero value is found, a message similar to that above is issued, and the user is sent to the CRDES Central Processor prompt.

Each "MK" partition coefficient section includes a "Methods Detail" subsection that details the CRD113 methods. Where applicable, and to the extent practical, their estimation methods in CRD113 are based on procedures suggested in the Superfund Exposure Assessment Manual<sup>6</sup>. With the exception of MKro, these coefficients are "time averaged" (see Section 2.2.3), and the time effect of applicable decay rate constant is incorporated into the coefficient.

### 11.1 Plant to Beef Partition Coefficient (Kpm)

Two options are available for estimating Kpm. The first option uses Kpat as a starting point; the estimate is  $Kpm = Kpat \times fm$ . The other option uses Kpd as a starting point; the estimate is  $Kpm = Kpd \times fm / fd$ . Option 1 requires Kpat input if CRDES3 is entered from OPEN3. Option 2 requires Kpd input if CRDES3 is accessed from OPEN3. Figure 31 demonstrates Kpm processing with CRDES3 entry from CHMF3. The non-chemical related data in this and subsequent figures are from DEFAULT.LDS.

**CAUTION:** If CRDES3 was accessed by entry mode 3 (from CHMF3 under DUST control) and option 2 is selected, the online value of Kpd is employed. Under DUST control, the Kpd subroutine follows the Kpm subroutine. If Kpd is incorrect, the estimated Kpm will be incorrect. If this happens, adjust Kpd under DUST control. At the conclusion of the DUST control routine, use option '6' within CHMF3 to again access the Kpm subroutine.

```

Press ENTER(return) key to continue...
***** Kpm ESTIMATION METHOD OPTIONS *****
      Enter value for desired method
Select '0' to exit without any calculation
Select '1' to estimate Kpm from Kpat
Select '2' to estimate Kpm from Kpd
Enter your selection:: 2
***** NON-CHEMICAL DATA ACCESSION SUBROUTINE *****
Last .LDS file downloaded was...
Last .LDS file operation was...
Last .LDS file stored was...
Title for online non-chemical data file is...
REVIEW OF .LDS FILES AVAILABLE ON disk 2 device \phas3\disk2\
Disk 1 device listed below
D:\PHAS3\DISK1
DEFAULT .LDS      DOWNLOAD.LDS
6492160 Bytes free

HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
Select '0' to exit without any selection
Select '1' to use DEFAULT.LDS non-chemical data
Select '2' to use non-chemical data from a .LDS file you select
Select '3' to use non-chemical data which are online.
Enter your selection:: 2
ENTER .LDS FILE (omit extension): download
Title for downloaded file is...
This is where information about a site whose properties are entered in the .LDS
file would be described.
86 fm, fat content in beef = .2
87 fd, fat content in milk = .04
214 Kpd, Plant (forage) to milk p.c., mg/L milk per mg/kg (dwb) = .0002
213 Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb) = .001
Estimate by method # 2
CHMF3 Online value is: .001
Replace online value with estimate? (yes/no):: yes

** CRDES3 Central Processor: Wish to do more in CRDES3?
Enter 'yes' or 'no': no
***** YOU HAVE RETURNED TO CHMF3 *****
Current value for
213 Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb) is .001
Current documentation message:: space for documentation in .DAT File item 213
Do you want to change documentation (yes/no)?:: no

```

Figure 31. Kpm Subroutine Display with CRDES3-CHMF3 Interface for Mode 2 Access.

## 11.2 Plant to Milk Partition Coefficient (Kpd)

Two options are available for estimating Kpd. They are "mirror images" of those used for Kpm, where fm and fd are switched in equations. The equations involved are:  $Kpd = Kpat \times fd$  and  $Kpd = Kpm \times fd / fm$ . If CRDES3 is entered from OPEN3, the user inputs either Kpat (option 1) or Kpm (option 2).

## 11.3 Soil to Water Partition Coefficient (Kd)

The routine estimates Kd from the relation  $Kd = foc \times Koc$ . There are five Kd soil selections that may be used in PHAS, and each may have a different foc associated with it. Thus, the first prompt is:

Which Kd do you want? (enter '1' for Kd1, '2' for Kd2, etc.)  
 Kd1 for #1 subsite pathways  
 Kd2 for #2 subsite pathways  
 Kd3 for basement subsoil  
 Kd4 for subsoil to outside diffusion/infiltration  
 Kd5 for sediment  
 Enter '0' to exit without calculation  
 Enter your selection::

After this prompt, the Non-Chemical Data Accession Subroutine menu appears. CAUTION: If CRDES3 was accessed from OPEN3: the user must know which foc corresponds to which subscript; see Table 3 for the dataname indices.

#### 11.4 Soil to Surface Water Runoff Coefficients (MKro1 and MKro2)

MKro1 or MKro2 indicate the mg/kg pollutant in soil at a contaminated site (subsite #1 or subsite #2) that will lead to 1 mg/L pollutant in a surface water body. In this section, the subsite designator is omitted. If CRDES3 was accessed via entry modes 1 or 2, following the CRDES3 Section Menu, the user must designate the subsite. This message appears:

For which subsite is MKro to be computed?  
 Enter '1' for subsite #1 - '2' for subsite #2  
 Enter your selection here::

If CRDES3 was accessed via entry mode 3, this designation step does not occur, and the method selection menu directly follows the information message.

Three methods are available to value these coefficients. Kd1 (or Kd2) is the only chemical-related datum required. The non-chemical data are obtained from a .LDS file as shown in Figure 31 and described above.

#### Methods Detail

The first method is the "adjusted" Kd model. Here,  $MKro = Kd + thav/rh$ . This equation assumes that all runoff water has attained equilibrium with contaminated soil, which can be considered the "worst case" situation.

The second method uses the relation:  $MKro = (Acw / Aw) \times (Kd + thav/rh)$ . This equation assumes that all the runoff water from the contaminated site attains equilibrium with contaminated soil as in the first method. However, the runoff water is "diluted" by clean water from non-contaminated portions of the surface water body watershed. The runoff water volume per unit area is the same in all parts of the watershed.

The third method is the "USLE-Haithé" approach. "USLE", the acronym for Universal Soil Loss Equation, is discussed in Section 2.4.3 of the Superfund Exposure Assessment Manual (SEAM)<sup>6</sup>. This empirical equation was developed by Wischmeier and Smith<sup>17</sup>, and provides an estimate of sediment runoff (SOILLD)\*.

\* Here, and in subsequent sections, the symbols used are either those shown in Table 3 or those used in program code.

In units of kg/year, this runoff is:

$$\text{SOILLD} = 2240 \text{ Acw} \times (K \times \text{LS} \times C \times P \times R)$$

Acw, K, LS, C and P are unique for a given watershed. The rain/runoff factor for a contaminated site (R) is used for an entire site. Factors have been determined for the United States East of the Rocky Mountains, and factor contours for that area appear in Figure 32.

The Haithe model<sup>18</sup> partitions pollutant between sediment and runoff. This model is based on a mass balance between rain and contaminated soil and assumes that the partitioning is restricted to the surface soil to a 1 cm depth. For convenience, a term  $\text{KFACT} = K_d \times r_h / (\text{FC} - \text{WP})$  is defined. Then, a 1 mg/kg pollutant concentration in topsoil provides a corresponding concentration in sediment (KSFACT) and in runoff water (KWFACT):

$$\begin{aligned}\text{KSFACT} &= \text{KFACT} / (1 + \text{KFACT}) \\ \text{KWFACT} &= 1 / (1 + \text{KFACT})\end{aligned}$$

The mg/year of pollutant in sediment carried off in runoff water is the product  $\text{SOILLD} \times \text{KSFACT}$ . The yearly runoff (RUNOF) in liters/year is:  $\text{RUNOF} = 1 \times 10^7 \text{ Acw} \times \text{RO} / 39.37$ . The coefficient converts from hectares to  $\text{m}^2$  and  $\text{m}^3$  to liters, while 39.37 converts meters to inches. Haithe<sup>18</sup> makes an "adverse case" assumption that all runoff water from the contaminated site attains the concentration KWFACT. Then, the dissolved pollutant transported in this runoff is the product  $\text{RUNOF} \times \text{KWFACT}$ . The total pollutant transported from a site is POLLOAD, which in mg/year, is

$$(\text{SOILLD} \times \text{KSFACT}) + (\text{RUNOF} \times \text{KWFACT})$$

PHAS3 includes another conservative assumption: the surface soil concentration of pollutant remains at 1 mg/kg. This differs from the presentation in SEAM<sup>6</sup>, and that of Haithe<sup>18</sup>.

As in the second method, there may be inputs of non-contaminated water to the surface water body. The yearly input of such water is called UPFLOW:

$$\text{UPFLOW} = 3.16 \times 10^{10} \text{ Qu}$$

In this equation,  $3.16 \times 10^{10}$  converts  $\text{m}^3/\text{sec}$  to liters/year. Then,  $\text{MKro} = (\text{UPFLOW} + \text{RUNOF}) / \text{POLLOAD}$ . Figure 33 is a sample of this method's display with CRDES3 accession mode '1'.

#### 11.5 Soil Flux Partition Coefficients (MKdb and MKdo)

These partition coefficients indicate the mg/kg in soil needed to produce a vapor flux of  $1 \text{ mg}/\text{m}^2\text{-day}$  from a uniformly contaminated area. As with MKro1 and MKro2, one subroutine handles both coefficients. The 'db' subscript refers to vapor diffusion in a basement, while the 'do' subscript refers to vapor diffusion to the outdoors. In terms of the diffusion from soil to air step per se, the methodology is similar for both coefficients.



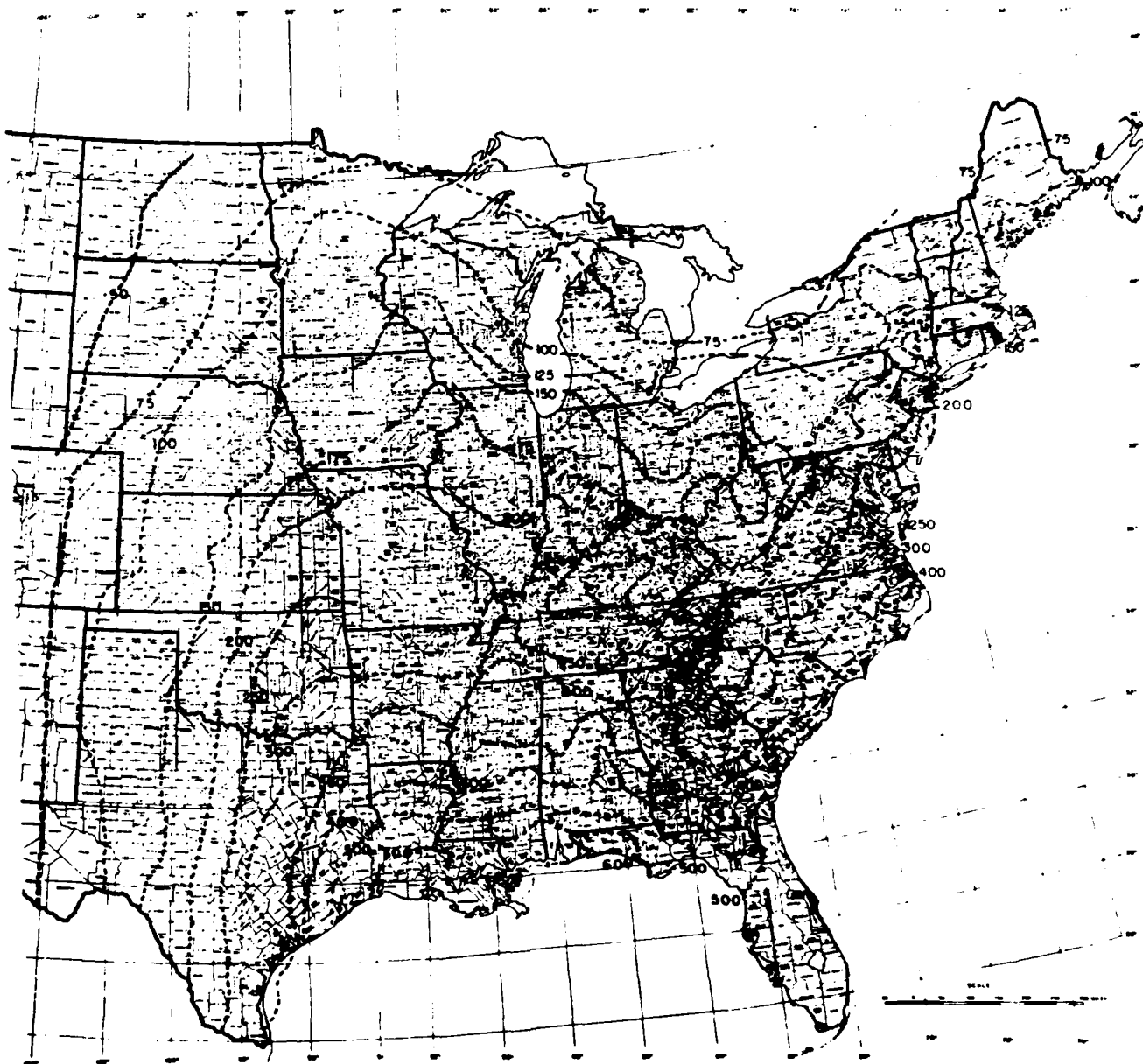


Figure 32. Rain/Runoff Factors for the Eastern United States<sup>17</sup>

If CRDES3 is accessed via entry mode 1 or 2, after the CRDES3 Selection Menu, the next display is:

```
Select an option for specific MK(diffusion):
Select '0' to skip selections
Select '1' for basement pathway and long-term exposure (MKdba)
Select '2' for basement pathway and short-term exposure (MKdbc)
Select '3' for outdoors pathway and long-term exposure (MKdoa)
Select '4' for outdoors pathway and short-term exposure (MKdoc)
Enter your selection here::
```

The chemical-related data inputs are Da, Kh, LPdss, and Kd3 (for MKdb) or Kd4 (for MKdo). Figure 34 shows the display where entry is from CHMF3.

```
***** MKro1 and MKro2 ESTIMATION METHOD OPTIONS *****
You are computing MKro1
NOTE: suffix for watershed site (1 or 2) is 'j'
Select '0' to exit this subroutine without calculation
Select '1' to compute MKroj as adjusted Kdj
Select '2' to compute MKroj as Kdj adjusted for watershed area;
      uses above data and total and contaminated watershed area data
Select '3' for 'USLE-Haith' approach for runoff & sediment
Enter your selection here:: 3

***** NON-CHEMICAL DATA ACCESSION SUBROUTINE *****
Last .LDS file downloaded was...
Last .LDS file operation was...
Last .LDS file stored was...
Title for online non-chemical data file is...
REVIEW OF .LDS FILES AVAILABLE ON disk 2 device \phas3\disk2\
Disk 1 device listed below
D:\PHAS3\DISK1
DEFAULT .LDS      DOWNLOAD.LDS
12187648 Bytes free

HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
Select '0' to exit without any selection
Select '1' to use DEFAULT.LDS non-chemical data
Select '2' to use non-chemical data from a .LDS file you select
Select '3' to use non-chemical data which are online.
Enter your selection:: 3

Enter KD Value:: 25
112 rh1, bulk density, topsoil #1 subsite, kg/L = 1.4
113 th1, average moisture capacity, topsoil #1 subsite, L/L = .1
114 Acw1, contaminated area of #1 subsite, ha = 10
116 WP1, wilt point, topsoil #1 subsite = .08
117 FC1, field capacity, topsoil #1 subsite = .25
118 K1, erodability factor for #1 subsite = .35
119 LS1, length-slope factor for #1 subsite = 1
120 C1, crop cover factor for #1 subsite = .12
121 P1, erosion control factor for #1 subsite = 1
122 R01, runoff from #1 subsite, inches/year = 8
123 Qul, Annual ave. flow above #1 subsite outfall, m^3/sec = .2
124 R1, rain/runoff factor for contaminated site = 150
231 MKro1, model soil/water p.c., #1 subsite runoff, mg/kg / mg/L = 26566.54
Estimate by method # 3

** CRDES3 Central Processor: Wish to do more in CRDES3?
Enter 'yes' or 'no'::
```

Figure 33. MKro1 Estimation by the USLE-Haith Approach. CRDES3 Access from OPEN3

```

Select an options for specific MK(diffusion):
Select '0' to skip selections
Select '1' for basement pathway and long-term exposure
Select '2' for basement pathway and short-term exposure
Select '3' for outdoors pathway and long-term exposure
Select '4' for outdoors pathway and short-term exposure
Enter your selection here:: 1

```

*(information message omitted)*

```

Press ENTER(return) key to continue...
***** NON-CHEMICAL DATA ACCESSION SUBROUTINE *****
Last .LDS file downloaded was...
Last .LDS file operation was...
Last .LDS file stored was...
Title for online non-chemical data file is...
REVIEW OF .LDS FILES AVAILABLE ON disk 2 device \phas3\disk2\
Disk 1 device listed below
D:\PHAS3\DISK1
DEFAULT .LDS      DOWNLOAD.LDS
12197888 Bytes free

HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....
Select '0' to exit without any selection
  (use for exit from this subroutine)
Select '1' to use DEFAULT.LDS non-chemical data
Select '2' to use non-chemical data from a .LDS file you select
Select '3' to use non-chemical data which are online.
Enter your selection:: 1
Title for downloaded file is...
Default file for starting new .LDS file. Check user's guide for parameter value
derivation.
You are computing MKdb-type term (basement)
Enter KD value:: 2
Enter Da value:: .55
Enter dimensionless Henry Law Constant:: .0003
Enter persistence rate constant LPdss for subsoil (1/year):: .0001
142 rh3, soil bulk density, basement model, kg/L = 1.8
143 th3, soil fraction voids with water, basement model, L/L = .15
144 ep3, soil fraction voids with air, basement model, L/L = .2
145 db, initial top of pollution layer below grade, basement model, m = .1
146 hb, lower depth of pollution layer, basement model, m = 3
77 Teta, Time exposure for adult, topsoil pathways, days = 10950
Washout time (days) = 2674977
233 MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m^2-day =
52.36946
Estimate by method # 1

** CRDES3 Central Processor: Wish to do more in CRDES3?
Enter 'yes' or 'no':

```

Figure 34. MKdba Estimation in CRD113. CRDES3 Access From OPEN3.

#### Method Details

The one-dimensional, unsteady state diffusion equation is:

$$\frac{\partial^2 C}{\partial z^2} = D \frac{\partial C}{\partial t}$$

where C is the concentration of pollutant in bulk soil (all phases), z is the depth dimension ( z is zero at the surface and increases with depth), D is a soil diffusivity, and t is time. C(z,t) is the function that is the solution to this equation, defined for positive time and position. The instantaneous surface flux Fn(t) is:

$$F_n(t) = D \times \left( \frac{\partial C(z,t)}{\partial z} \right)_{z=0}$$

The time-averaged flux,  $F_{av}(t)$ , is sought, from which the corresponding  $MK(\text{diffusion}) = 1/F_{av}(t)$ . The closed-form expression for  $F_{av}(t)$  includes  $F_n(t)$  and accounts for the persistence rate constant  $LP_{dss}$

$$F_{av}(t) = (1/t) \int_0^t F_n(t) \times \exp(-LP_{dss} \times t) dt \quad (11)$$

The method in CRD113 provides an approximation to equation 11. The Farino adaptation of the Thibodeaux and Hwang equation discussed in SEAM, Section 2.3.2.1.(4)<sup>6</sup> is first discussed. It computes a time-averaged flux without accounting for  $LP_{dss}$ . Their equation is based on the following assumptions:

- (1) only one-dimensional flux to the surface via the air phase is addressed (water-phase diffusion can be neglected).
- (2) At time zero in the analysis, the pollutant is uniformly 1 mg/kg in a soil layer that starts at depth  $db$  (for  $MK_{db}$  coefficients) or  $do$  (for  $MK_{do}$  coefficients) below the surface and extends downwards to depth  $hb$  (for  $MK_{db}$  coefficients) or  $ho$  (for  $MK_{do}$  coefficients).
- (3) The concentration of the pollutant in air immediately above the soil surface is initially zero.
- (4) In the contaminated soil layer, equilibrium is established between the substance in soil, soil water, and the air in soil voids.
- (5) Isothermal conditions prevail in the soil column.
- (6) No other mechanism of pollution depletion occurs, nor is the soil column physically disturbed.

The analysis exposure period ends at time  $T_{Eta}$  or  $T_{Etc}$ . In the equations that follow, the exposure period is called  $t_f$ . For convenience, these terms are defined (subscripts for the basement situation).

$$KDA = K_{d3} + th_3/rh_3$$

$$DEI = (Kh \times Da \times ep_3^{10/3}) / (th_3 + ep_3)^2$$

$$KDJJ = rh_3 \times KDA + th_3 + Kh \times ep_3$$

$DEI$  is similar to the "phase transfer coefficient" of equation 2-12 in SEAM<sup>6</sup>. However, the Millington-Quirk porosity adjustment term is used here rather than the  $ep^{4/3}$  term suggested in SEAM<sup>6</sup>. The author considers the SEAM treatment as unnecessarily conservative.  $KDJJ$  corresponds to the term  $C_S/C_B$  in equations 2-11 and 2-14 in SEAM<sup>6</sup>.

First, a dryout time,  $TTYME$  is computed:

$$TTYME = KDJJ \times (hb^2 - db^2) / (2 DEI).$$

If  $TTYME < t_f$ , the pollutant is essentially stripped from the soil layer before the end of the exposure period. In that case, this message appears:

Washout time (days) <TTYME> used in calcs.

If TTYME > tf, a message appears indicating the washout time in days (see Figure 34). The average flux is:

$$Favn(tf) = 2000 DEI / (KDA \times [db + SQRTERM^{0.5}]) \quad (12a)$$

$$\text{where } SQRTERM = db^2 + 2(DEI \times tf / KDJJ). \quad (12b)$$

A corollary expression is derived from the definition of a time-averaged functions (see equation 9 for an equation in terms of intake):

$$\int_{t1}^{t2} F_n(t) dt = t2 \times Favn(t2) - t1 \times Favn(t1) \quad (13)$$

Referring back to equation 11, the time interval from 0 to tf can be integrated in increments; one such increment is t1 to t2,  $t2 \leq tf$ . If time intervals are reasonably short, the exponent term of equation 11 is nearly constant. In each such interval, such as the interval ending at  $t_i$ , the exponent term is approximated as  $ETERM_i$ , where

$$ETERM_i = \exp(-0.5(t_{i-1} + t_i) LPdss) \quad (14)$$

and can be removed from the integral. Equation 11 then is approximated:

$$Favn(tf) = [1/tf] [ETERM_{t1} \int_0^{t1} F_n(t) dt + \dots ETERM_{i-1} \int_{t_{i-1}}^{t_i} F_n(t) dt + \dots ETERM_n \int_{t_{n-1}}^{tf} F_n(t) dt]$$

Equation 13 is used to evaluate each integral, and after  $ETERM_i$  is evaluated according to equation 14, the result is:

$$Fav(tf) = (1/tf) \sum_{i=1}^n \exp[-0.5(t_i + t_{i-1}) LPdss] \times [t_i \times Favn(t_i) - (t_{i-1}) \times Favn(t_{i-1})] \quad (15)$$

Where  $Favn(t)$  is evaluated from equations 12a and 12b. Details on the time increment algorithm used in CRD113 appear in Appendix B, Section B.8.4.

#### 11.6 Sediment Flux Partition Coefficient (MKdw)

MKdw indicates the mg/kg in sediment needed to produce a pollutant in water flux of  $1 \text{ mg/m}^2\text{-day}$  from an uniformly contaminated area. The CRD113 method employs the chemical-related data inputs  $Kd5$ ,  $Dw$ , and  $LPsed$ . If CRDES3 was accessed by entry mode 1 or 2, after the CRDES3 Selection Menu display, this display message appears:

```
Select time frame for analysis... Select '0' to quit without estimation
Select '1' for long-term exposure, select '2' for short-term exposure
Enter your selection here::
```

If CRDES3 was accessed by entry mode 3, this message is omitted, and the next display is the information message. Figure 35 demonstrates the MKdwa subroutine display for entry mode 3 (data processing is under DUST control).

\*\*\*\*\* CHMF3 DUST CONTROL OF DATA PROCESSING ROUTINE \*\*\*\*\*  
237 MKdwa, sediment/openwater p.c. long-term, mg/kg per mg/m<sup>2</sup>-day = 1567.391

Documentation: space for documentation in .DAT File item 237  
Main input variable to intake pathway eqtn.  
Select '1' to accept current value.  
Select '2' to replace value  
Select '3' to directly access dataname info/estimation subroutine.  
Estimation routine available.  
Select '4' to replace documentation message  
Enter your selection:: 3

(information message omitted)

Press ENTER(return) key to continue...

\*\*\*\*\* NON-CHEMICAL DATA ACCESSION SUBROUTINE \*\*\*\*\*

Last .LDS file downloaded was...

Last .LDS file operation was...

Last .LDS file stored was...

Title for online non-chemical data file is...

REVIEW OF .LDS FILES AVAILABLE ON disk 2 device \phas3\disk2\

Disk 1 device listed below

D:\PHAS3\DISK1

DEFAULT .LDS            DOWNLOAD.LDS

12193792 Bytes free

HERE ARE NON-CHEMICAL DATA ACCESSION OPTIONS.....

Select '0' to exit without any selection

(use for exit from this subroutine)

Select '1' to use DEFAULT.LDS non-chemical data

Select '2' to use non-chemical data from a .LDS file you select

Select '3' to use non-chemical data which are online.

Enter your selection:: 1

Title for downloaded file is...

Default file for starting new .LDS file. Check user's guide for parameter value derivation.

222 LPsed, persistence rate constant for sediment, 1/year = .001

79 TEsa, Time exposure for adults, sediment pathways, days = 10950

219 Kd5 sediment/water p.c., mg/kg / mg/L = 50

207 Dw, Molecular diffusivity in water, m<sup>2</sup>/sec = .000055

102 rh5, bulk density of sediment, kg/L = 1.5

103 th5, void fraction of sediment, L/L = .4

104 dp5, initial top of pollution layer in sediment below grade, m = .5

105 hp5, bottom depth of pollution layer in sediment below grade, m = 5

Washout time (days) = 5.756262E+07

237 MKdwa, sediment/openwater p.c. long-term, mg/kg per mg/m<sup>2</sup>-day = 1581.301

Estimate by method # 1

CHMF3 Online value is: 1567.391

Replace online value with estimate? (yes/no):: no

\*\* CRDES3 Central Processor: Wish to do more in CRDES3?

Enter 'yes' or 'no':: no

\*\*\*\*\* CHMF3 DUST CONTROL OF DATA PROCESSING ROUTINE \*\*\*\*\*

237 MKdwa, sediment/openwater p.c. long-term, mg/kg per mg/m<sup>2</sup>-day = 1567.391

Documentation: space for documentation in .DAT File item 237

Main input variable to intake pathway eqtn.

Select '1' to accept current value.

Figure 35. MKdwa Estimation in CRD113. Access from CHMF3 Under DUST Control

### Method Details

The method in CRD113 is similar to that discussed for MKdb and MKdo in Section 11.5, except that diffusion is from sediment to water and the persistence rate constant LPsed is involved. Thus, this section deals only with the diffusion equation for FavN. The rest of the details in Section 11.5 apply, with LPsed substituted for LPdss. The diffusion equation is based on these assumptions:

(1) Only one-dimensional flux to the sediment surface-water bottom interface is considered.

(2) At the initial time for analysis, the pollutant is at a uniform concentration of 1 mg/kg in the sediment layer. The layer starts at a depth below sediment grade  $dp_5$  and extends downwards to a depth  $hp_5$ .

(3) The concentration of pollutant at the sediment-water interface is initially zero.

(4) In the contaminated sediment layer, equilibrium is established between the substance in sediment and water in sediment voids.

(5) Other mechanisms leading to pollutant loss from sediment or sediment scouring by open water turbulence are not addressed.

(6) Isothermal conditions prevail throughout the exposure period.

For convenience, these terms are defined:

$$\begin{aligned} KDJ &= KD_5 + th_5 / rh_5 \\ KDJJ &= rh_5 \times KDJ \\ DEI &= DW \times th_5^{4/3} \end{aligned}$$

As with MKdb or MKdo, a washout time is calculated:

$$TTYME = (KDJJ \times [hp_5^2 - dp_5^2]) / (2 DEI)$$

The subroutine checks to see if  $TES_a$  or  $TES_c$ , whichever is applicable, exceeds  $TTYME$ ; the shortest of the comparison times is used in calculations. If  $TTYME$  is shorter, this message appears: " Washout time (days) "  $\langle TTYME \rangle$  " used in calcs." As in the previous section, the exposure time in the computation is called  $tf$ .

The average flux is computed as

$$Favn(tf) = 2000DEI / (KDJ \times [dp_5 + SQRTERM^{0.5}])$$

where  $SQRTERM = dp_5^2 + (2 DEI \times tf / KDJJ)$ .

#### 11.7 Groundwater Infiltration Partition Coefficient (MKgw)

MKgw indicates the mg/kg in topsoil or near surface soil required to produce 1 mg/L in groundwater. In the CRD113 subroutine,  $Kd_4$  and  $LPdss$  are the chemical-related data. When CRDES3 is accessed via entry mode 1 or 2, after the CRDES3 Selection Menu, this selection display appears:

```
Select time frame for analysis... Select '0' to quit without estimation
Select '1' for long-term exposure, select '2' for short-term exposure
Enter your selection here::
```

If CRDES3 was accessed by entry mode 3, this message is omitted, and the next display is the information message. Figure 36 shows a sample display for MKgwa computed for mode 1 entry to CRDES3.

Select time frame for analysis... Select '0' to quit without estimation  
 Select '1' for long-term exposure, select '2' for short-term exposure  
 Enter your selection here:: 1

(information message omitted)  
 (DEFAULT LDS downloaded)

Title for downloaded file is...  
 Default file for starting new LDS file. Check user's guide for parameter value derivation.

Enter Kd4 value:: 5  
 Enter persistence rate constant LPdss (1/year):: .01  
 153 rh4, soil bulk density, outside diffusion, kg/L = 1.8  
 158 AO4, area of site for outside diffusion/infiltration, ha = 10  
 163 TH6, pollutant thickness in soil column (groundwater infiltration), m = 10  
 164 RI6, infiltration of rainwater to aquifer, m/year = .1  
 165 VGW6, velocity of groundwater flow, m/year = 365  
 166 TAQ6, thickness of aquifer, m = 10  
 167 th6, effective porosity in aquifer, L/L = .35  
 77 Teta, Time exposure for adult, topsoil pathways, days = 10950  
 239 MKgwa, topsoil/groundwater p.c. long-term, mg/kg per mg/L = 2445895  
 Estimate by method # 1

\*\* CRDES3 Central Processor: Wish to do more in CRDES3?  
 Enter 'yes' or 'no'::

Figure 36. MKgwa Estimation in CRD113. CRDES3 Access From OPEN3.

#### Method Details

The method in CRD113 computes the mass of pollutant removed from a contaminated soil layer via its transfer to rainwater that infiltrates to the aquifer (infiltrate). The transfer is time-averaged since the amount of pollutant available for removal continues to decrease as time progresses. This method proceeds in time increments steps, and the impact of pollutant persistence is factored in. Assumptions made are:

- (1) Infiltration is uniform throughout the year.
- (2) Kd4 relates the concentrations of pollutant in soil and infiltrate.
- (3) Infiltrate is thoroughly mixed with groundwater in the aquifer prior to groundwater use for domestic purposes.
- (4) The area contaminated, AO4, is the same area as is involved in outside diffusion, and does not diminish in extent as time progresses.
- (5) The removal of pollutant from the unsaturated soil column by diffusion to outdoor air or runoff is neglected. This is a conservative assumption.
- (6) Within each step time interval, the concentration of pollutant in soil remains constant. Changes in concentration are assessed between steps.
- (7) Any dispersion or retardation effects during transport to a down-gradient domestic water user are ignored. This is a conservative assumption.



(8) The groundwater flows under the area AO4 at a uniform speed. The area AO4 is approximately square, and flow is directed normal to two opposite sides of the square.

(9) There is no further reduction of pollutant in groundwater due to environmental effects.

Initially, the pollutant concentration in soil is 1 mg/kg. The pollutant mass in a segment TK6 m deep per unit area in the soil column ( $\text{mg/m}^2$ ) is  $\text{MASSINT}(0) = 1000 \times \text{TK6} \times \text{rh4}$ . Since TK6 is in meters and rh4 is in kg/L, the 1000 factor converts from  $\text{m}^3$  to liters.

The calculation is carried out in time interval steps; for convenience, the total time duration is called  $t_f$ . The first time interval is shortest of one year (365.25 days),  $25.3/\text{LPdss}$  days (where LPdss is in  $\text{years}^{-1}$ , or the exposure time specified. A mass balance after the first interval expresses the pollutant mass retained in soil,  $\text{MASSINT}(1)$ , in terms of  $\text{MASSINT}(0)$ :

$$\text{MASSINT}(1) = [\text{MASSINT}(0) - (1000 \times \text{INF} \times \text{Cw}(1))] \times \exp(-\text{LPdss} \times t_1)$$

where  $\text{Cw}$  refers to pollutant concentration in infiltrate ( $\text{mg/L}$ ).  $\text{INF}$  is the infiltrate in the time period; see assumption (1) above. The 1000 converts  $\text{m}^3$  to L.  $\text{Cw}$  is linked to soil concentration through  $\text{Kd4}$ . Since  $\text{Cs}(0) = 1 \text{ mg/kg}$ ,  $\text{Cw}(1) = 1/\text{Kd4}$ . Then,  $\text{MASSINT}(1)$  can be computed. From the unit concentration assignment,  $\text{Cs}(1) = \text{MASSINT}(1)/\text{MASSINT}(0)$ , and mass of pollutant removed by infiltration,  $\text{MASSOUT}(1)$  is given as:

$$\text{MASSOUT}(1) = 1000 \times \text{INF} \times \text{AO4} \times \text{Cw}(1).$$

This procedure is iterated for subsequent intervals through the exposure time,  $t_f$ . In time intervals after the first, the exponent term becomes  $\exp(-\text{LPdss} \times (t_i - t_{i-1}))$ . In the  $i$ th interval,  $\text{MASSINT}(i)$  is computed based on the previous residual mass  $\text{MASSINT}(i-1)$ , and  $\text{Cs}(i) = \text{MASSINT}(i)/\text{MASSINT}(0)$ . If the time interval is based on LPdss, the time interval duration is adjusted as described in Appendix B, Section B.8.4. However, if the time interval for an iteration from this procedure would exceed one year, the interval is set to one year.

The summation of all  $\text{MASSOUT}(i)$  is called SUMMGW. The volume of infiltrate in liters throughout the entire process is VOLINF, and

$$\text{VOLINF} = 10^7 \times \text{RI6} \times \text{AO4} \times t_f/365.25.$$

This volume is "diluted" by groundwater. The dilution occurs in a section of aquifer of depth TAQ6 and width LOA, where  $\text{LOA} = 100 \text{ AO4}^{0.5}$  (TAQ6 and LOA are in m). In  $t_f/365.25$  years, the volume of groundwater in liters passing through this section is VOLAQF:

$$\text{VOLAQF} = 10^3 \text{ LOA} \times \text{th6} \times \text{TAQ6} \times \text{VGW6} \times t_f/365.25$$

MKGW is the inverse of pollutant concentration in the groundwater plume, or  $\text{MKGW} = (\text{VOLAQF} + \text{VOLINF}) / \text{SUMMGW}$ .

## 12.0 REFERENCES

For purposes of brevity in PHAS3 information files, several frequently-cited references appear in condensed form or as acronyms. The acronyms are listed below with either full references or cross-indexed with references in Section 12.1.

**DEAME** (Versar-EPAC 68024254/T170). Versar, Inc. 1989. Exposure Assessment Methods Handbook. Revised Draft Report for U.S. Environmental Protection Agency Contract 68-02-4254, Task 170. Versar, Inc., Springfield, VA.

**EFH89** (EPA 600/8-89/043). Exposure Assessment Group, Office of Health and Environmental Assessment. 1989. Exposure Factors Handbook. EPA/600/8-89/043. U.S. Environmental Protection Agency, Washington, DC

**FOSS**, Foth 7th. Foth, H.D. 1984. Fundamentals of Soil Science. John Wiley & Sons, New York, NY

**Lyman et al.**, CPEN. See reference 9, Section 12.1

**McKone87** (EST 1194-1201). See reference 19, Section 12.1

**Perry83** (NTIS PB83-177659). See reference 7, Section 12.1

**PPLVM** (TR8918, DTIC AD-A206976). See reference 14, Section 12.1.

**RAGS1-IF89** (EPA/540/1-89-002. See reference 2, Section 12.1.

**RAGS1-SUPP91**, (OSWER 9285.6-03, PB91-921314). See reference 3, Section 12.1.

**SEAM88** (EPA/540/1-88-001). See reference 6, Section 12.1.

**SPHEM85** (OSWER 9285.1, EPA 540/1-88-060). Office of Emergency and Remedial Response. 1986. Superfund Public Health Evaluation Manual. EPA 540/1-86-060. United States Environmental Protection Agency, Washington, DC

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13. Garten, C.T., Jr. and J.R. Trabalka. 1983. Evaluation of models for predicting terrestrial food chain behavior of xenobiotics. Environ. Sci. Technol. 17:590-595.
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18. Haith, D.A. 1980. A mathematical model for estimating pesticide losses in runoff. J. Environ. Qual. 9(3):428-433.

19. McKone, T.E. 1987. Human exposure to volatile organic compounds in tap water: the indoor inhalation pathway. Environ. Sci. Technol. 21(12):1194-1201

## 12.2 References Cited Only in PHAS3 Information Files

The following references are cited in PHAS3 display messages, but not in the text. After the reference, the first file in alphabetical order that cites the reference is presented. All .CMP files precede .NCI files. These files can be read by any word-processing program that handles ASCII files.

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APPENDIX A. GLOSSARY OF TERMS, ACRONYMS, AND DATANAMES IN MAIN TEXT

Table A-1. Frequently-Used Terms and Acronyms.

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Continuation return - Use of the return (enter key) to continue program operation.

.DAT - Extension for chemical-specific data files.

data - numerical values used in intake or constraint equations.

dataname - title used in PHAS3 to describe a specific datum.

Disk 1 device - The magnetic storage hardware or subdirectory partition thereof that contains PHAS3 executable programs and supplemental files.

Disk 2 device - The magnetic storage hardware or subdirectory partition thereof that contains PHAS3 external files and files developed by the user.

DOS - Disk Operating System for IBM personal computers and compatible hardware systems (for example: Microsoft MS-DOS, Version 5.0).

download - A verb; act of moving data or information from a file in storage to program memory.

downloaded - An adjective; to describe file contents that have been copied to program memory.

DUST - Data Use Status Table. This is a numerical list, where each element indicates the role or status in a scenario of the dataname with the same index.

DUST control - use of the DUST from a .PXX file to restrict the data processing program presentations of data to only those items relevant to the scenario in the .PXX file.

dwb - Dry weight basis

EPA - U.S. Environmental Protection Agency

External file - A portion of the disk 2 device reserved for specific information or data stored for use in PHAS3 programs. Each file has a unique filename.

Filename - The identification for a file in PHAS3.

index - A number which identifies a particular element of an array.

information - numerical values or text used for purposes other than as inputs to PHAS3 equations.

.LDS - Extension for non-chemical specific data files.

medium - a repository of a pollutant in the environment that is subject to remediation. Thus, the user may process pathways involving exposure via water when soil is the definitive medium.

online - capable of being transferred between PHAS3 programs (programmers refer to data or information with this attribute as COMMON or GLOBAL)

p.c. - partition coefficient

PHAS3 - Pollutant Hazard Assessment System, this version.

PHLD - Public Health Limit Dose. A dose which serves as a criterion for assessment purposes. Typical units are mg/kg body weight-day

PPLV - Preliminary Pollutant Limit Value. In the water and sediment media, the medium concentration corresponding to a hazard index of one for a specific pollutant and scenario.

.PXX - Generic extension for scenario information files. The specific names are, by medium: for sediment - .PSD, for topsoil - .PTS, and for water - .PWA.

RAGS - Risk Assessment Guidance for Superfund. Volume I- Human Health Evaluation Manual, Part A.<sup>2</sup>

SEAM - Superfund Exposure Assessment Manual<sup>6</sup>

SST - Scenario Selection Table. This is a numeric list, where each element indicates whether a certain pathway is included in a scenario, and depending on the medium, provides optional pathway selections.

.STO - Extension for Scenario Data Needs Report files.

Table A-2. Datanames and Symbols Used in PHAS3. (page 1 of 4 pages)

Identification of Dataname (Alphabetical Order)	Index
Ab3, basement area contacting soil diffusing vapors, m <sup>2</sup>	148
Acw1, contaminated area of #1 subsite, ha	114
Acw2, cont. area for watershed #2 site, ha	129
AFsa, Time adjustment factor, long-term (adult), sediment paths	65
AFsc, Time adjustment factor, short-term (child), sediment paths	66
Afta, Time adjustment factor, long-term (adult), topsoil paths	63
Aftc, Time adjustment factor, short-term (child), topsoil paths	64
AFwa, Time adjustment factor, long-term (adult), water paths	61
AFwc, Time adjustment factor, short-term (child), water paths	62
AO4, area of site for outside diffusion/infiltration, ha	158
AQTL, Aquatic toxicity limit in water, mg/L	243
As5, surface area of contaminated sediment in waterway, ha	106
Aw1, total watershed area at #1 subsite outfall, ha	115
Aw2, total watershed area at #2 subsite outfall, ha	130
BAF, Fish bioaccumulation factor, mg/kg fish per mg/L	210
BCF, Fish Bioconcentration [in water] factor, mg/kg fish per mg/L	198
BIRa, adult inhalation rate, basement vapors, m <sup>3</sup> /day	18
BIRc, child inhalation rate, basement vapors, m <sup>3</sup> /day	43
BWa, adult body weight, kg	1
BWc, child body weight, kg	26
BWD, representative dairy cow body weight, kg	95
BWM, representative steer body weight, kg	94
C1, crop cover factor for #1 subsite	120
C2, crop cover factor for #2 subsite	135
CSI, construction area-related dust intake, kg/workday	17
CTAEL, Cattle toxicity adverse effects limit, mg/kg-day	247
CWTF, weather/time factor for construction site soil pathway	53
Da, Molecular diffusivity in air, m <sup>2</sup> /sec	206
DAWa, adult body surface for dermal exposure to water, m <sup>2</sup>	4
DAWc, child body surface for dermal exposure to water, m <sup>2</sup>	29
db, initial top of pollution layer below grade, basement model, m	145
DETa, adult dermal exposure time to domestic water, hr/day	5
DETC, child dermal exposure time to domestic water, hr/day	30
do, initial top of pollution layer below grade, outside diffusion, m	156
dp5, initial top of pollution layer in sediment below grade, m	104
DTdl, Long-term limit dose estimate, dermal basis, mg/kg-day	180
DTds, Short-term limit dose estimate, dermal basis, mg/kg-day	181
DTil, Long-term limit dose estimate, inhalation basis, mg/kg-day	178
DTis, Short-term limit dose estimate, inhalation basis, mg/kg-day	179
DTol, Long-term limit dose estimate, oral basis, mg/kg-day	176
DTos, Short-term limit dose estimate, oral basis, mg/kg-day	177
Dw, Molecular diffusivity in water, m <sup>2</sup> /sec	207
DW4, distance from site to off-site receptors, m	161
EIRa, adult inhalation rate, offsite residential, m <sup>3</sup> /day	19
EIRc, child inhalation rate, offsite residential, m <sup>3</sup> /day	44
EIWa, adult oral water equiv. for inhaled pollutants, L/day	3
EIWc, child water oral water equiv. for inhaled pollutant, L/day	28



Table A-2. Datanames and Symbols Used in PHAS3. (page 2 of 4 pages)

Identification of Dataname (Alphabetical Order)	Index
ep3, soil fraction voids with air, basement model, L/L	144
ep4, soil fraction voids with air, outside diffusion, L/L	155
FC1, field capacity, topsoil #1 subsite	117
FC2, field capacity, topsoil #2 subsite	132
fd, fat content in milk	87
fm, fat content in beef	86
foc for soil used to determine soil/veg p.c.	195
foc for soil used to determine soil/forage p.c.	196
foc1, fraction organic carbon, topsoil #1 subsite	111
foc2, fraction organic carbon, topsoil #2 subsite	126
foc3, soil fraction organic carbon, basement model	141
foc4, soil fraction organic carbon, outside diffusion	152
foc5, fraction organic carbon content of sediment	101
focPS, foc for soil used to determine phytotoxicity limit	246
hb, lower depth of pollution layer, basement model, m	146
ho, lower depth of pollution layer, outside diffusion, m	157
hp5, bottom depth of pollution layer in sediment below grade, m	105
IWa, adult drinking water intake, L/day	2
IWc, child drinking water intake, L/day	27
K1, erodability factor for #1 subsite	118
K2, erodability factor for #2 subsite	133
Kd1 soil/water p.c. for #1 subsite pathways, mg/kg / mg/L	215
Kd2 soil/water p.c. for #2 subsite pathways, mg/kg / mg/L	216
Kd3 soil/water p.c. for basement subsoil, mg/kg / mg/L	217
Kd4 soil/water p.c. for outside diffusion, mg/kg / mg/L	218
Kd5 sediment/water p.c., mg/kg / mg/L	219
Kh, Henry Law constant, dimensionless [conc./conc.]	208
Koc, Organic carbon/water p.c., mg/L per mg/kg (OC)	192
Kpat, Plant (forage) to adipose tissue p.c., mg/kg per mg/kg dwb	197
Kpd, Plant (forage) to milk p.c., mg/L milk per mg/kg (dwb)	214
Kpm, Plant (forage) to meat p.c., mg/kg meat per mg/kg (dwb)	213
Ksp, Soil/plant (forage) p.c., mg/kg (dwb) per mg/kg soil	194
Ksv, Soil/vegetable p.c., mg/kg (dwb) per mg/kg soil	193
Kwp, Water to plant (forage) p.c., mg/kg (dwb) per mg/L	212
Kwv, Water to vegetable p.c., mg/kg (dwb) per mg/L	211
LogP, Log (base10) octanol-water partition coefficient	188
LPds, persistence rate constant for diffusion-layer subsoils, 1/year	225
LPsed, persistence rate constant for sediment, 1/year	222
LPTs1, persistence rate constant for #1 subsite soil, 1/year	223
LPTs2, persistence rate constant for #2 subsite soil, 1/year	224
LPwat, persistence rate constant for surface water, 1/year	221
LS1, length-slope factor for #1 subsite	119
LS2, length-slope factor for #2 subsite	134
MH, rep. mixing height, on-site, m	160
MH4, rep. mixing height for off-site receptor, m	162
MKdba, soil flux p.c., basement model long-term, mg/kg per mg/m <sup>2</sup> -day	233
MKdbc, soil flux p.c., basement model short-term, mg/kg per mg/m <sup>2</sup> -day	234

Table A-2. Datanames and Symbols Used in PHAS3. (page 3 of 4 pages)

Identification of Dataname (Alphabetical Order)	Index
MKdoa, soil flux p.c., outdoors long-term, mg/kg per mg/m <sup>2</sup> -day	235
MKdoc, soil flux p.c., outdoors short-term, mg/kg per mg/m <sup>2</sup> -day	236
MKdwa, sediment/openwater p.c. long-term, mg/kg per mg/m <sup>2</sup> -day	237
MKdwc, sediment/openwater p.c. short-term, mg/kg per mg/m <sup>2</sup> -day	238
MKgwa, topsoil/groundwater p.c. long-term, mg/kg per mg/L	239
MKgwc, topsoil/groundwater p.c. short-term, mg/kg per mg/L	240
MKrol, model soil/water p.c., #1 subsite runoff, mg/kg / mg/L	231
MKro2, model soil/water p.c., #2 subsite runoff, mg/kg / mg/L	232
MW, Molecular weight, g/mol	186
MXb, dilution air factor for vapor flux in basement, day/m <sup>3</sup>	171
MXef, windblown particle rate to offsite receptors, kg/m <sup>2</sup> -day	174
MXof, dilution air factor for vapor flux off-site, day/m <sup>3</sup>	173
MXon, dilution air factor for vapor flux to outside on-site, day/m <sup>3</sup>	172
ODTa, adult water activity immersion time, hour/TA day	8
ODTc, child water activity immersion time, hr/TA day	33
OIRa, adult inhalation rate, onsite residential, m <sup>3</sup> /day	16
OIRc, child inhalation rate, onsite residential, m <sup>3</sup> /day	41
OIwa, swimwater ingested by adult, L/TA day	6
OIwc, swimwater ingested by child, L/TA day	31
ORwa, adult inhalation rate during water activity, m <sup>3</sup> /TA day	7
ORwc, child inhalation rate for water activity, m <sup>3</sup> /TA day	32
P1, erosion control factor for #1 subsite	121
P2, erosion control factor for #2 subsite	136
PC, Dermal permeability constant, cm/hr	209
PEF, soil particulate inhalation efficiency factor	55
PHLS, Phytotoxicity limit in soil, mg/kg	245
PHLW, Phytotoxicity limit in water, mg/L	244
PLa, adult perspiration rate, L/m <sup>2</sup> /day	15
PLc, child perspiration rate, L/m <sup>2</sup> /day	40
Qa3, volume air through basement, m <sup>3</sup> /day	147
Qu1, Annual ave. flow above #1 subsite outfall, m <sup>3</sup> /sec	123
Qu2, Annual ave. flow above #2 subsite outfall, m <sup>3</sup> /sec	138
Qu5, annual flow of waterway below polluted sediment locale, m <sup>3</sup> /sec	107
R1, rain/runoff factor for contaminated site	124
rh1, bulk density, topsoil #1 subsite, kg/L	112
rh2, bulk density, topsoil #2 subsite	127
rh3, soil bulk density, basement model, kg/L	142
rh4, soil bulk density, outside diffusion, kg/L	153
rh5, bulk density of sediment, kg/L	102
RI6, infiltration of rainwater to aquifer, m/year	164
RO1, runoff from #1 subsite, inches/year	122
RO2, runoff from #2 subsite, inches/year	137
RSPA, particulate conc in air, residential, kg/m <sup>3</sup>	52
SARa, adult exposure area to dust on skin, residential, m <sup>2</sup>	14
SARc, child exposure area to dust on skin, residential, m <sup>2</sup>	39
SIRa, adult oral intake of soil, residential, kg/day	13
SIRc, child oral intake of soil, residential, kg/day	38
SLA, soil loading rate on exposed skin, kg/m <sup>2</sup> /day	51

Table A-2. Datanames and Symbols Used in PHAS3. (page 4 of 4 pages)

Identification of Dataname (Alphabetical Order)	Index
TAF, Long-term averaging time adjustment code	185
TAQ6, thickness of aquifer, m	166
Tb, Normal or extrapolated boiling point, deg C	190
TEca, Time exposure for adults, construction pathway, days	74
TEsa, Time exposure for adults, sediment pathways, days	79
TEsc, Time exposure for child, sediment pathways, days	80
TEta, Time exposure for adult, topsoil pathways, days	77
TEtc, Time exposure for child, topsoil pathways, days	78
TEwa, Time exposure for adults, water pathways, days	75
TEwc, Time exposure for child, water pathways, days	76
th1, average moisture capacity, topsoil #1 subsite, L/L	113
th2, average moisture capacity, topsoil #2 subsite, L/L	128
th3, soil fraction voids with water, basement model, L/L	143
th4, soil fraction voids with water, outside diffusion, L/L	154
th5, void fraction of sediment, L/L	103
th6, effective porosity in aquifer, L/L	167
TK6, pollutant thickness in soil column (groundwater infiltration), m	163
Tm, Normal or extrapolated melting point, deg C	187
TOL, Organoleptic limit - taste in water, mg/L	241
Upd, plant (forage) intake by dairy cow, kg (dwb)/day	92
Upm, plant (forage) intake by steer, kg (dwb)/day	89
Usd, soil intake by dairy cow, kg/day	93
Usm, soil intake by steer, kg/day	90
UW3, wind-speed for on-site exposure to diffusing vapors, m/sec	151
UW4, wind-speed for off-site exposure to diffusing vapors, m/sec	159
Uwd, water intake by dairy cow, L/day	91
Uwm, water intake by steer, L/day	88
VGW6, velocity of groundwater flow, m/year	165
VP, Saturated vapor pressure, mm Hg	191
Wda, adult milk consumption, L/day	12
Wdc, child dairy consumption, L/day	37
WECF, wind erosion climatic factor, unitless	54
Wfa, adult fish consumption, kg/day	9
Wfc, child fish consumption, kg/day	34
Wma, adult beef consumption, kg/day	11
Wmc, child beef consumption, kg/day	36
WP1, wilt point, topsoil #1 subsite	116
WP2, wilt point, topsoil #2 subsite	131
Wsol, Water solubility, mg/L	189
Wva, adult vegetable consumption, kg dwb/day	10
Wvc, child vegetable consumption, kg/day	35

## APPENDIX B. PATHWAY AND CONSTRAINT EQUATIONS

Appendix B presents the unit intake equations that are used in COMP3 as well as the constraint equations in CONTS and CONWS. Refer to Table A-2 in Appendix A for dataname symbols. Section B.1 identifies special variable names used in intake and constraint equations. Section B.2 contains assumption statements for intake equations, each preceded by a letter. After each intake equation in Sections B.3 through Sections B.5, assumptions implied in the equation are identified by statement letters from Section B.2. The pathway titles are those displayed in PATWAY3 or COMP3. Sections B.6 and B.7 provide the algorithms for Type 1 and Type 2 Constraint tests. Section B.8 discusses the derivation of dataname values in DEFAULT.LDS that could not be documented fully within on-line information capacity and time increments for super partition coefficient estimations in CRD113 subroutines.

In addition to the assumptions listed in Section B.2, there are assumptions associated with "super" partition coefficients computed in NOCH3 and CRDES3. The sections of main text that discuss these coefficients are:

<u>Datanames</u>	<u>Text Section</u>
MXb	6.4.1
MXon	6.4.2
MXof	6.4.3
MXef	6.4.4
MKro	11.4
MKdb, MKdo	11.5
MKdw	11.6
MKgw	11.7

### B.1 SPECIAL TERMS USED IN EQUATIONS

CFIO = DTol/DTil for adults or DTos/Dtis for children. CFIO was defined in Section 2.2, "Dermal and Respired Pollutant Intake". In that section, the ratios are expressed in terms of PHLD, while here the term DT is used.

CFDO = DTol/DTdl for adults or DTos/DTds for children.

FDL =  $2.5 (Dw/86400)^{-2/3}$  The constant 2.5 is the cube root of the ratio of air to water viscosity at 20 °C. The constant 86400 converts days to seconds.

FDA =  $((1/Kh) \times [Da/86400])^{-2/3}$  The constant 86400 converts days to seconds.

KDJ1 = Kd1 + th1/rh1.

PCEF =  $2.9 \times 10^6$  ; this is FDL for perchloroethylene, see Section B.8.1.

### B.2 ASSUMPTIONS IMPLIED IN PATHWAY INTAKE EQUATIONS

a. Differences in consumption rates between nominal daily intakes (oral intake per day of either liquid, food or soil and inhaled air) and pathway intakes are accounted for by the "AF" adjustment factors (dataname indices 61-66).

- b. The inhaled intake of pollutant can be accounted for by an equivalent oral intake of pollutant, which is called EIWa for an adult and EIWc for a child. This equivalent oral intake is based on a model proposed by McKone<sup>19</sup>, and is discussed in Section B.8.1. In PHAS3, EIWa and EIWc are based on model results for perchloroethylene, and values for other pollutants are scaled to these results by the fraction  $PCEF/(FDA+FDL)$ .
- c. The absorption of pollutant through skin occurs at a constant rate.
- d. The concentration of a highly volatile substance in air is related to its solubility in water by the Henry Law Constant, Kh. The concentration of pollutant above open water is a function of Henry's Law and terms related to the ease of mass transfer of pollutant through air and water interfaces.
- e. The volume of water is sufficient to cover skin at all times through the exposure period.
- f. The pollutant content of all vegetables relative to pollutant content in water can be represented by the partition coefficient Kwv.
- g. Cows absorb pollutant with equal efficiency from water, forage or soil.
- h. The pollutant content of any forage relative to pollutant content in water can be represented by the partition coefficient Kwp.
- i. When water is the environmental medium, plants obtain pollutant primarily from water applied to crops or pasture as opposed to soil-water.
- j. The same Kwp can be used for livestock and dairy cows.
- k. In the topsoil medium pathways, vegetables and forage plants obtain pollutant from pollutant in soil solution (which is the water referred to in the Kwv or Kwp term). An equilibrium exists between pollutant in soil and soil solution expressed by KDJ1.
- l. The factor SLA is the same for adults and children.
- m. When pollutant is absorbed from soil on the skin, the pollutant initially in soil that contacts skin is partitioned between soil and perspiration. All pollutant in perspiration is transported through the skin.
- n. The inhalation and skin absorption components of exposure are included in an augmented oral ingestion term.
- o. The exponential argument LP term, indicating the persistence of pollutant in soil or sediment, is resolved within the formulation of the "MK" partition coefficient.

### B.3 WATER RELATED PATHWAYS

The generic term  $TCF = 1/PERK \times (1 - \exp[-PERK])$ , where PERK represents either PERKa or PERKc.  $PERKa = TEWa \times LPwat$ ;  $PERKc = TEWc \times LPwat$ . See Section B.8.2 for further details.

PATHWAY 1 ingest water with pollutant from domestic supply

$$\begin{aligned}\text{INTAKE} &= \text{IWa} \times \text{AFwa} \times \text{TCFa} && (\text{adult}) \\ \text{INTAKE} &= \text{IWc} \times \text{AFwc} \times \text{TCFc} && (\text{child})\end{aligned}$$

Assumptions: a

PATHWAY 2 inhale pollutant volatilized from household water (all uses)

$$\begin{aligned}\text{INTAKE} &= \text{EIWa} \times \text{CFIO} \times \text{TCFa} \times \text{AFwa} \times \text{PCEF}/(\text{FDA}+\text{FDL}) && (\text{adult}) \\ \text{INTAKE} &= \text{EIWc} \times \text{CFIO} \times \text{TCFc} \times \text{AFwc} \times \text{PCEF}/(\text{FDA}+\text{FDL}) && (\text{child})\end{aligned}$$

Assumptions: a, b.

PATHWAY 3 dermal absorption of pollutant from contact with household water.

$$\begin{aligned}\text{INTAKE} &= 10 \times \text{DAWa} \times \text{DETa} \times \text{PC} \times \text{CFDO} \times \text{AFwa} \times \text{TCFa} && (\text{adult}) \\ \text{INTAKE} &= 10 \times \text{DAWc} \times \text{DETC} \times \text{PC} \times \text{CFDO} \times \text{AFwc} \times \text{TCFc} && (\text{child})\end{aligned}$$

The constant 10 accounts for  $\text{m}^2$  to  $\text{cm}^2$  and  $\text{cm}^3$  to L conversions. This constant also appears in the pathway 6 equation below and, for other media, in pathway 3 and pathway 6 equations.

Assumptions: a, c, e

PATHWAY 4 ingest water with pollutant while in water sport/play activity.

$$\begin{aligned}\text{INTAKE} &= \text{OIWa} \times \text{AFwa} \times \text{TCFa} && (\text{adult}) \\ \text{INTAKE} &= \text{OIWc} \times \text{AFwc} \times \text{TCFc} && (\text{child})\end{aligned}$$

Assumptions: a

PATHWAY 5 inhale vaporized pollutant from open water during water activity.

$$\begin{aligned}\text{INTAKE} &= 1000 \times \text{ORWa} \times \text{AFwa} \times \text{TCFa} \times \text{CFIO} \times \text{Kh} \times \text{FDL}/(\text{FDL}+\text{FDA}) && (\text{adult}) \\ \text{INTAKE} &= 1000 \times \text{ORWc} \times \text{AFwc} \times \text{TCFc} \times \text{CFIO} \times \text{Kh} \times \text{FDL}/(\text{FDL}+\text{FDA}) && (\text{child})\end{aligned}$$

The constant 1000 converts from  $\text{m}^3$  to L. This also applies to pathway 5 equations for other media.

Assumptions: a, d

PATHWAY 6 absorb pollutant through skin while in water activity.

$$\begin{aligned}\text{INTAKE} &= 10 \times \text{DAWa} \times \text{ODTa} \times \text{AFwa} \times \text{TCFa} \times \text{PC} \times \text{CFDO} && (\text{adult}) \\ \text{INTAKE} &= 10 \times \text{DAWc} \times \text{ODTC} \times \text{AFwc} \times \text{TCFc} \times \text{PC} \times \text{CFDO} && (\text{child})\end{aligned}$$

Assumptions: a, c, e.

PATHWAY 7 consume fish from contaminated water.

$$\begin{aligned}\text{INTAKE} &= \text{Wfa} \times \text{BCF} \times \text{AFwa} \times \text{TCFa} && (\text{adult}) \\ \text{INTAKE} &= \text{Wfc} \times \text{BCF} \times \text{AFwc} \times \text{TCFc} && (\text{child})\end{aligned}$$

Assumptions: a

Pathway 8 consume vegetables watered with contaminated water.

INTAKE =  $Wva \times Kwv \times AFwa \times TCfa$  (adult)  
INTAKE =  $Wvc \times Kwv \times AFwc \times TCfc$  (child)

Assumptions: a,f

PATHWAY 9 consume beef, livestock drinks contaminated water (first option).

INTAKE =  $Wma \times Kpm \times (Uwm/Upm) \times AFwa \times TCfa$  (adult)  
INTAKE =  $Wmc \times Kpm \times (Uwm/Upm) \times AFwc \times TCfc$  (child)

Assumptions: a,g

PATHWAY 9 consume beef, livestock drinks contaminated water and grazes on plants irrigated with contaminated water (second option).

INTAKE =  $Wma \times Kpm \times [(Uwm/Upm) + Kwp] \times AFwa \times TCfa$  (adult)  
INTAKE =  $Wmc \times Kpm \times [(Uwm/Upm) + Kwp] \times AFwc \times TCfc$  (child)

Assumptions: a,g,h,i

PATHWAY 10 drink milk, dairy cows drink contaminated water (first option).

INTAKE =  $Wda \times Kpd \times (Uwd/Upd) \times AFwa \times TCfa$  (adult)  
INTAKE =  $Wdc \times Kpd \times (Uwd/Upd) \times AFwc \times TCfc$  (child)

Assumptions: a,g,j

PATHWAY 10 drink milk, dairy cows drink contaminated water and graze on plants irrigated with contaminated water (second option).

INTAKE =  $Wda \times Kpd \times [(Uwd/Upd) + Kwp] \times AFwa \times TCfa$  (adult)  
INTAKE =  $Wdc \times Kpd \times [(Uwd/Upd) + Kwp] \times AFwc \times TCfc$  (child)

Assumptions: a,g,h,i,j

#### B.4 SURFACE SOIL RELATED PATHWAYS

In pathways where subsite #1 or subsite #2 designation must be specified, the equation for subsite #1 is presented. The generic term TCF is defined as  $(1 - \exp[-PERK]) / PERK$  where PERK represents either PERKa or PERKc.  
 $PERKa = Teta \times LPts1$  and  $PERKc = Tetc \times LPts1$ .

PATHWAY 1 ingest water with pollutant from domestic supply; pollutant in runoff from topsoil of #1 subsite.

INTAKE =  $IWa \times Afta \times TCfa / MKrol$  (adult)  
INTAKE =  $IWc \times Aftc \times TCfc / MKrol$  (child)

Assumptions: a

PATHWAY 2 inhale pollutant volatilized from household water (all uses);  
pollutant in runoff from topsoil of #1 subsite.

INTAKE =  $(1/MKrol) \times EIWa \times Afta \times TCfa \times CFIO \times PCEF / (FDA + FDL)$  (adult)  
INTAKE =  $(1/MKrol) \times EIWc \times AFTc \times TCfc \times CFIO \times PCEF / (FDA + FDL)$  (child)

Assumptions: a, b

PATHWAY 3 dermal absorption of pollutant from contact with household water;  
pollutant in runoff from topsoil of #1 subsite.

INTAKE =  $(10/MKrol) \times DAWa \times DETa \times PC \times CFDO \times Afta \times TCfa$  (adult)  
INTAKE =  $(10/MKrol) \times DAWc \times DETc \times PC \times CFDO \times Aftc \times TCfc$  (child)

Assumptions: a, c, e

PATHWAY 4 ingest water with pollutant while in water sport/play activity;  
pollutant in runoff from topsoil of designated <#1 or #2 subsite>.

INTAKE =  $OIWa \times Afta \times TCfa / MKrol$  (adult)  
INTAKE =  $OIWc \times Aftc \times TCfc / MKrol$  (child)

Assumptions: a

PATHWAY 5 inhale vaporized pollutant from open water during water activity;  
pollutant in runoff from topsoil of designated <#1 or #2 subsite>.

INTAKE =  $(1000/MKrol) \times ORWa \times CFIO \times Afta \times TCfa \times Kh \times FDL / (FDL + FDA)$  (adult)  
INTAKE =  $(1000/MKrol) \times ORWc \times CFIO \times Afta \times TCfa \times Kh \times FDL / (FDL + FDA)$  (child)

Assumptions: a, d

PATHWAY 6 absorb pollutant through skin while in water activity; pollutant in  
runoff from topsoil of designated <#1 or #2 subsite>.

INTAKE =  $(10/MKrol) \times DAWa \times ODTa \times PC \times CFDO \times Afta \times TCfa$  (adult)  
INTAKE =  $(10/MKrol) \times DAWc \times ODTc \times PC \times CFDO \times Aftc \times TCfc$  (child)

Assumptions: a, c, e

PATHWAY 7 consume fish from contaminated water; pollutant is in runoff from  
topsoil of designated <#1 or #2 subsite>.

INTAKE =  $Wfa \times BAF \times Afta \times TCfa / MKrol$  (adult)  
INTAKE =  $Wfc \times BAF \times Aftc \times TCfc / MKrol$  (child)

Assumptions: a

PATHWAY 8 consume contaminated vegs. grown at designated <#1 or #2 subsite>.

INTAKE =  $Wva \times Kwv \times Afta \times TCfa / KDJ1$  (adult)  
INTAKE =  $Wvc \times Kwv \times Aftc \times TCfc / KDJ1$  (child)

Assumptions: a, f, k



PATHWAY 9 consume beef, livestock grazes on forage grown at designated <#1 or #2 subsite>, first of three options.

$$\begin{aligned} \text{INTAKE} &= Wma \times Kpm \times Kwp \times Afta \times TCfa / KDJ1 && (\text{adult}) \\ \text{INTAKE} &= Wmc \times Kpm \times Kwp \times Aftc \times TCfc / KDJ1 && (\text{child}) \end{aligned}$$

Assumptions: a,h,k

PATHWAY 9 consume beef, livestock grazes on forage grown at designated <#1 or #2 subsite>, second of three options. Allowance is made for livestock ingestion of soil.

$$\begin{aligned} \text{INTAKE} &= Wma \times Kpm \times Afta \times TCfa \times (Kwp/KDJ1 + Usm/Upm) && (\text{adult}) \\ \text{INTAKE} &= Wmc \times Kpm \times Aftc \times TCfc \times (Kwp/KDJ1 + Usm/Upm) && (\text{child}) \end{aligned}$$

Assumptions: a,g,h,k

PATHWAY 9 consume beef, livestock grazes on forage grown at designated <#1 or #2 subsite>, third of three options. Allowance is made for livestock ingestion of soil and for livestock watering on surface supply which gets cont. runoff from subsite. Adult and child intake equation are, respectively:

$$\begin{aligned} \text{INTAKE} &= Wma \times Kpm \times Afta \times TCfa \times (Kwp/KDJ1 + Usm/Upm + Uwm/[Upm \times MKro1]) && (\text{adult}) \\ \text{INTAKE} &= Wmc \times Kpm \times Aftc \times TCfc \times (Kwp/KDJ1 + Usm/Upm + Uwm/[Upm \times MKro1]) && (\text{child}) \end{aligned}$$

Assumptions: a,g,h,k

PATHWAY 10 drink milk, dairy cows graze on forage grown at designated <#1 or #2 subsite>, first of three options.

$$\begin{aligned} \text{INTAKE} &= Wda \times Kpd \times Kwp \times Afta \times TCfa / KDJ1 && (\text{adult}) \\ \text{INTAKE} &= Wdc \times Kpd \times Kwp \times Aftc \times TCfc / KDJ1 && (\text{child}) \end{aligned}$$

Assumptions: a,h,j,k

PATHWAY 10 drink milk, dairy cows graze on forage grown at designated <#1 or #2 subsite>, second of three options. Allowance is made for dairy cow ingestion of soil.

$$\begin{aligned} \text{INTAKE} &= Wda \times Kpd \times Afta \times TCfa \times (Kwp/KDJ1 + Usd/Upd) && (\text{adult}) \\ \text{INTAKE} &= Wdc \times Kpd \times Aftc \times TCfc \times (Kwp/KDJ1 + Usd/Upd) && (\text{child}) \end{aligned}$$

Assumptions: a,g,h,j,k

PATHWAY 10 drink milk, dairy cows graze on forage grown at designated <#1 or #2 subsite>, third of three options. Allowance is made for dairy cow ingestion of soil and for animals watering on surface supply which gets cont. runoff from subsite. Adult and child intake equations are, respectively:

$$\begin{aligned} \text{INTAKE} &= Wda \times Kpd \times Afta \times TCfa \times (Kwp/KDJ1 + Usd/Upd + Uwd/[Upd \times MKro1]) && (\text{adult}) \\ \text{INTAKE} &= Wdc \times Kpd \times Aftc \times TCfc \times (Kwp/KDJ1 + Usd/Upd + Uwd/[Upd \times MKro1]) && (\text{child}) \end{aligned}$$

Assumptions: a,g,h,j,k

PATHWAY 11 exposure to dirt at residence (oral, dermal, respired).

INTAKE = Afta x TCfa x (SIRa+[SARa x PLa x CFDO x MGPCc]+[OIRa x RSPA x CFIO]) (adult)

INTAKE = Aftc x TCfc x (SIRc+[SARc x PLc x CFDO x MGPCc]+[OIRc x RSPA x CFIO]) (child)

MGPCc = SLA/(SLAxKDJ1 + PLa) for adults; for children, SLA/(SLAxKDJ1 + PLc) .

MGPCc is the mg/L pollutant in perspiration water per mg/kg pollutant initially in soil deposited on skin. MGPCc is derived from two equations reflecting partitioning between soil and perspiration, and a pollutant mass balance between these substrates.

Assumptions: a,c,l,m.

PATHWAY 12 exposure to dirt at occupational site (adults only).

INTAKE = CSI x (TEca/TEta) x CWTF x TCF2

Site is assumed to be at assigned subsite #1.

Assumptions: a,n

PATHWAY 13 exposure to vapors diffusing from soil in vicinity of house.

Exposure assumed to be primarily caused by inhalation of vapors in basement.

INTAKE = BIRa x Afta x CFIO x Ab3 x MXb/MKdba (adult)

INTAKE = BIRc x Aftc x CFIO x Ab3 x MXb/MKdbc (child)

Assumptions: a,o

PATHWAY 14 exposure to vapors diffusing from soil outside of house.

Exposure assumed to be primarily caused by inhalation of diffusing vapors.

INTAKE = 10000 EIRa x Afta x CFIO x AO4 x MXon/MKdoa (adult)

INTAKE = 10000 EIRc x Aftc x CFIO x AO4 x MXon/MKdoc (child)

The constant 10000 converts ha to m<sup>2</sup>; also applies to pathway 15.

Assumptions: a,o.

PATHWAY 15 exposure to vapors diffusing from soil at site and to windblown particles from site to offsite receptors.

INTAKE = 10000 EIRa x Afta x CFIO x AO4 x MXof x (<sup>MKef</sup>[PEFxWCEP]+1/MKdoa) (adult)

INTAKE = 10000 EIRc x Aftc x CFIO x AO4 x MXof x (<sup>MKef</sup>[PEFxWCEP]+1/MKdoc) (child)

Assumptions: a,o

PATHWAY 16 ingest water with pollutant from domestic supply; pollutant infiltrates through soil to groundwater source.

INTAKE = IWa x Afta/MKgwa (adult)

INTAKE = IWc x Afta/MKgwc (child)

Assumptions: a,o

PATHWAY 17 inhale pollutant volatilized from household water (all uses);  
pollutant infiltrates through soil to groundwater source.

INTAKE =  $(1/\text{MKgwa}) \times \text{AFta} \times \text{EIWa} \times \text{CFIO} \times \text{PCEF}/(\text{FDA}+\text{FDL})$  (adult)

INTAKE =  $(1/\text{MKgwc}) \times \text{AFtc} \times \text{EIWc} \times \text{CFIO} \times \text{PCEF}/(\text{FDA}+\text{FDL})$  (child)

Assumptions: a,b,o

PATHWAY 18 dermal absorption of pollutant from contact with household water;  
pollutant infiltrates through soil to groundwater source.

INTAKE =  $(10/\text{MKrol}) \times \text{DAWa} \times \text{DETa} \times \text{PC} \times \text{CFDO} \times \text{AFta}$  (adult)

INTAKE =  $(10/\text{MKrol}) \times \text{DAWc} \times \text{DEtc} \times \text{PC} \times \text{CFDO} \times \text{AFtc}$  (child)

The constant 10 accounts for  $\text{m}^2$  to  $\text{cm}^2$  and  $\text{cm}^3$  to L conversions.

Assumptions: a,c,e,o

#### B.5 SEDIMENT-RELATED PATHWAYS

PATHWAY 1 ingest water with pollutant from domestic supply. Water source  
has been in contact with polluted sediment.

INTAKE =  $\text{IWa} \times \text{AFsa}/\text{MKdwa}$  (adult)

INTAKE =  $\text{IWc} \times \text{AFsc}/\text{MKdwc}$  (child)

Assumptions: a,o

PATHWAY 2 inhale pollutant volatilized from household water (all uses)  
Water source has been in contact with polluted sediment.

INTAKE =  $(1/\text{MKdwa}) \times \text{EIWa} \times \text{AFsa} \times \text{CFIO} \times \text{PCEF}/(\text{FDA}+\text{FDL})$  (adult)

INTAKE =  $(1/\text{MKdwc}) \times \text{EIWc} \times \text{AFsc} \times \text{CFIO} \times \text{PCEF}/(\text{FDA}+\text{FDL})$  (child)

Assumptions: a,b,o

PATHWAY 3 dermal absorption of pollutant from contact with household water  
Water source has been in contact with polluted sediment.

INTAKE =  $(10/\text{MKdwa}) \times \text{DAWa} \times \text{DETa} \times \text{PC} \times \text{CFDO} \times \text{AFsa}$  (adult)

INTAKE =  $(10/\text{MKdwc}) \times \text{DAWc} \times \text{DEtc} \times \text{PC} \times \text{CFDO} \times \text{AFsc}$  (child)

Assumptions: a,b,e,o

PATHWAY 4 ingest water with pollutant while in water sport/play activity  
Waterbody overlays a polluted sediment site.

INTAKE =  $\text{OIWa} \times \text{AFsa}/\text{MKdwa}$  (adult)

INTAKE =  $\text{OIWc} \times \text{AFsc}/\text{MKdwc}$  (child)

Assumptions: a,o

PATHWAY 5 inhale vaporized pollutant from open water during water activity  
Waterbody overlays a polluted sediment site.

INTAKE =  $(1000/MKdwa) \times ORWa \times AFsa \times CFIO \times Kh \times FDL/(FDL+FDA)$  (adult)  
INTAKE =  $(1000/MKdwc) \times ORWc \times AFsc \times CFDO \times Kh \times FDL/(FDL+FDA)$  (child)

Assumptions: a,b,e,o

PATHWAY 6 absorb pollutant through skin while in water activity. Waterbody  
overlays a polluted sediment site.

INTAKE =  $10 \times DAWa \times ODTa \times AFsa \times PC \times CFDO/MKdwa$  (adult)  
INTAKE =  $10 \times DAWc \times ODTc \times AFsc \times PC \times CFDO/MKdwc$  (child)

Assumptions: a,b,e,o

PATHWAY 7 consume fish from contaminated water. Waterbody overlays a polluted  
sediment site.

INTAKE =  $Wfa \times AFsa \times BCF / MKdwa$  (adult)  
INTAKE =  $Wfc \times AFsc \times BCF / MKdwc$  (child)

Assumptions: a,b,i

#### B.6 TYPE 1 CONSTRAINT EQUATIONS

Each "TEST" is compared to the PPLV (water and sediment medium) or the  
applicable public health soil limit. If TEST is greater, a Type 1 constraint  
is identified.

##### Organoleptic Effects

Water	TEST = TOL
Sediment	TEST = $TOL \times 8640 \times Qu5 \times MKdwc/As5$ (*)
Soil	
Subsite #1	TEST = $TOL \times MKrol$
Subsite #2	TEST = $TOL \times MKro2$
Subsoil	TEST = $TOL \times MKgwc$

##### Adverse Effects to Aquatic Biota

Water	TEST = AQTL
Sediment	TEST = $AQTL \times 8640 \times Qu5 \times MKdwc/As5$ (*)
Soil	
Subsite #1	TEST = $AQTL \times MKrol$
Subsite #2	TEST = $AQTL \times MKro2$

\* The constant 8640 accounts for three unit conversions:  $1000 \text{ L/m}^3$ ,  $1 \text{ ha}/10^4 \text{ m}^2$ , and 86400 sec/day.

### Phytotoxicity

Note that two TEST terms can be proposed, one based on a limit from plants grown in water and one based on a limit from plants grown in soil.

Water	TEST = PHLW and TEST = PHL/(Koc x focPS)
Soil	
Subsite #1	TEST = PHLW x KDJ1; KDJ1 = Kd1 + th1/rh1 TEST = PHL x KDJ1/(Koc x focPS)
Subsite #2	TEST = PHLW x KDJ2; KDJ2 = Kd2 + th2/rh2 TEST = PHL x KDJ2/(Koc x focPS)

### Adverse Effects to Livestock or Dairy

Only the livestock-based equations are shown. The dairy-based equations are the same with substitution of BWD for BWM, Kpd for Kpm, Upd for Upm, etc.

Water: Option 1 is intake from water only. Option 2 includes intake from forage.

Option 1	TEST = CTael x BWM/Uwm
Option 2	TEST = CTael x BWM/(Uwm + [Upm x Kwp])

Soil: Option 1 is intake from forage only. Option 2 include intake from soil ingestion. Option 3 includes soil ingestion and intake from water contaminated by surface runoff. Only subsite #1 equations are shown. Replace "1" suffix with "2" to form analog subsite #2 equations.

Option 1	TEST = CTael x BWM/(Upm x Kwp/KDJ1)
Option 2	TEST = CTael x BWM/([Upm x Kwp/KDJ1] + Usm)
Option 3	TEST = CTael x BWM/([Upm x Kwp/KDJ1] + Usm + [Uwm/MKrol])

### B.7 Type 2 Constraints

The Type 2 constraint test for the water medium is straightforward: if the PPLV exceeds Wsol (limit of solubility in water), a Type 2 constraint is identified. If sediment is the medium, the term  $PPLV/(Kd5+th5/rh5)$  is compared to Wsol. If Wsol is exceeded, a Type 2 constraint is identified.

Type 2 constraint analysis for the soil medium is done on a pathway-by-pathway basis. The test for a given pathway starts with a conversion of the public health soil limit (See Figure 21; PHL) for the specified soil portion to a corresponding aqueous concentration (WSTEST). A Type 2 constraint occurs when WSTEST exceeds Wsol.

The equations presented below for pathways 1 through 11 are for the "#1 subsite"; those of pathways 4 through 10 for the "#2 subsite" are formed by substitution of the "1" suffix for the "2" suffix.

Pathways 1 - 7: WSTEST = PHL1/MKrol

Pathways 8 - 11: WSTEST = PHL1/KDJ1

A second WSTEST fraction, PHSL/MKro , could be included for the third option of pathway 9 or 10. This is not done. Practically speaking, the PHSL/KDJ term is smaller than PHSL/MKro ; thus if a Type 2 constraint does not occur with PHSL/KDJ , it won't occur with the other term.

There is no type 2 constraint associated with Pathway 12 intake.

Pathway 13: WSTEST = PHSL3/KDJ3

Pathway 14 and 15: WSTEST = PHSL4/KDJ4

Pathways 16-18: WSTEST = PHSL4/KDJ4

## B.8 SPECIAL TOPICS

### B.8.1 EIWa and EIWc values in DEFAULT.LDS

These values are evaluated according to treatment advanced by McKone<sup>19</sup>. In his model, the concentration of a volatile pollutant is computed for three compartmental parts of a house: the shower, the bathroom, and the rest of the house. Moreover, a "rest of the house compartment" average concentration is determined for the time periods, 7 AM to 11 PM and 11 PM to 7 AM. Specific activities leading to exposure are assigned to time periods. The inhaled intake of the pollutant is then the summation of all products

Activity time x Concentration x Inhalation Rate x Uptake efficiency

for each activity in a specific house compartment.

McKone<sup>19</sup> computes concentrations for a 1 mg/L content of pollutant in water. In McKone's<sup>19</sup> development, a key step in this process is to compute the transfer efficiency (VTE) of a pollutant relative to a highly volatile substance. He selected radon. For purposes of this section, a highly volatile pollutant, whose concentrations have been computed, can be used in place of radon if FDL+FDA is evaluated. Perchloroethylene (PCE) is selected, for which FDL>>>FDA, and FDL =  $2.9 \times 10^6$ . McKone indicates (his equation 19):

$$VTE_i = VTE_j \times (FDL+FDA)_j / (FDL + FDA)_i$$

In light of the above discussion, if "j" is perchloroethylene

$$VTE_i / VTE_j = PCEF / (FDL+FDA)_i$$

Transfer efficiency is directly related to concentration. Thus, the term  $PCEF / (FDL+FDA)_i$  scales concentration for other pollutants relative to that attained with PCE.

Computed PCE concentrations from McKone and intake data are listed in Table B-1. EIWa, the sum of adult intake factors, is 3.36 mg/day. EIWc factors are also listed in Table B-1. The author has modified some of McKone's values of time and inhalation rate to closely approximate a two-year old child (McKone defines an "infant" as 0-2 years of age, and a "child" as 2-16 years of age.) The computed EIWc is 1.05 mg/day.

TABLE B-1. Data Used to Estimate EIW Factors in DEFAULT.LDS

EIWA Factors

Function	Time min/day	Concentration mg/L of PCE	Inhalation Rate L/min	Intake, mg/day
Shower	10	$1.7 \times 10^{-2}$	20	1.70
Sleep	480	$2.3 \times 10^{-5}$	6.6	0.04
Bathroom use	40 <sup>1</sup>	$3.4 \times 10^{-3}$	20	1.36
Other activities	240 <sup>2</sup>	$1.1 \times 10^{-4}$	20	0.26

EIWc Factors

Function	Time min/day	Concentration mg/L of PCE	Inhalation Rate L/min	Intake, mg/day
Shower	5 <sup>3</sup>	$1.7 \times 10^{-2}$	7	0.298
Sleep	480	$2.3 \times 10^{-5}$	2.8	0.015
Bathroom use	40 <sup>1</sup>	$3.4 \times 10^{-3}$	7	0.476
Other activities	675 <sup>4</sup>	$1.1 \times 10^{-4}$	7	0.260

1. McKone<sup>19</sup> assumes 20 minutes bathroom use between 7-9 AM and 20 minutes at other times. An average pollutant concentration in bathroom air is listed by McKone<sup>19</sup> for the 7-9 AM time period, and is higher than for other times. The assumption here is that all bathroom use occurs from 7-9 AM.

2. McKone<sup>19</sup> assumes that adults are home for 4 hours between 7 AM to 11 PM. However, this includes time spent in the shower and in the bathroom. Here, "other activities" time remains 240 minutes.

3. The author equates a "shower" to a "bath". McKone<sup>19</sup> assumes that children spend 20 minutes/week showering. The author believes this is low, and generation of vapors in a bath should be less than from a shower. A shower time of 5 minutes/day is assumed by the author.

4. McKone<sup>19</sup> assumes that a 2- to 16-year old child spends 60 percent of time from 7 AM to 11 PM at home; and an infant is always at home during this time period. Here, a compromise time of 675 minutes is used, which is 75 percent of 960 minutes less time for bathroom and shower functions.

**B.8.2 Time-Averaged Functions**

With a first order decay process, the pollutant concentration at any time,  $C(t)$  equals  $C_0 \exp(-kt)$ , where  $C_0$  is the initial concentration,  $k$  is the first-order decay rate constant and  $t$  is time. The time averaged concentration over the period from zero to time  $t_f$ ,  $C_{av,t_f}$ , is defined as:

$$C_{av,t_f} = 1/t_f \int_0^{t_f} C(t) dt$$

Substitution and removal of constant terms outside the integral yields

$$Cav_{tf} = C_o/tf \int_0^{tf} \exp(-k \times t) dt$$

The integral can be evaluated in closed form:

$$Cav_{tf} = (C_o/[k \times tf]) (1-\exp[-k \times tf])$$

Let  $PERK = k \times tf$ , and if  $C_o = 1 \text{ mg/kg}$ ,

$$Cav_{tf} = (1/PERK) \times (1-\exp[-PERK])$$

Note that if  $(k \times tf) \ll 1$ , the  $(1-\exp[-PERK])$  term converges to  $(k \times tf)$ , and  $Cav_{tf}$  converges to 1.

#### B.8.3 Derivation of MGPCC for Pathway Equation 11

For the adult, SLA is the soil in contact with  $1 \text{ m}^2$  of skin daily. If the concentration of pollutant in that soil is  $1 \text{ mg/kg}$ , the pollutant available for transfer to that skin area is at most SLA. The pollutant distribution is subject to a mass balance:  $SLA = C_L \times PLA + C_S \times SLA$ , where  $C_L$  and  $C_S$  are pollutant in perspiration and soil. The distribution is assumed also subject to soil-liquid partitioning such that  $C_S = KDJ \times C_L$ , where KDJ is the soil-water partition coefficient. These equations are solved for  $C_L$ , which is called MGPCC in the equation.

#### B.8.4 Time Intervals to Estimate MK-Partition Coefficients

The discussion here is restricted to LPdss. The algorithm used in CRD113 starts with an incremental time interval of 1/10th the half life, converted to days. This time interval is called THK:

$$THK = 25.3/LPdss$$

when LPdss is in years. The first interval for calculation is then from zero to THK days. This procedure is repeated for 19 such intervals, at which the elapsed time is  $506/LPdss$  days. At this point, THK is increased to  $50.6/LPdss$  days. The time interval is increased by an additional  $25.3/LPdss$  days after each 20 intervals.

As the products within the summation of equation 14 are evaluated, the program checks two conditions: (1) the total time elapsed does not exceed  $tf$ , and (2) that the interval product term is not becoming vanishingly small. If either condition exists, the process is terminated, and the summation at that point computes  $Fav(tf)$ .



## APPENDIX C. SPECIAL PHAS3 ERROR TRAPS AND THEIR RESOLUTION

One user-friendly feature of PHAS3 is use of error traps. A trap interferes with the BASIC interpreter's default processing of a "fatal error", where BASIC detects an improper program command, and causes program termination or a "crash" with a terse explanation. Each trap diagnoses the probable cause of error and suggests corrective action. The main text discussed traps designed to detect user's improper file input errors, and in those cases, a "crash" is avoided. Section C.1 discusses error traps in OPEN3 which are triggered due to improper disk device assignments or deployment.

Errors that can't be resolved or easily diagnosed are trapped and the following generic message is issued:

Unexpected fatal error in <program> <error number> at <program line>. Please contact programmer at 301-619-2014 and provide details. Exiting from PHAS3 to DOS.

Referring to Table 2 in the text, disk 1 device files with extensions other than .BAS can be downloaded during PHAS3 operation. Moreover, the disk 2 device files cited in Section 4.3 can be downloaded. All supplied PHAS3 files are read-only, and should not be subject to deletion with DOS or most word-processing software. In most cases, if a file specified for downloading is missing, PHAS3 will crash. Section C.2 discusses the most likely crash scenarios due to missing files and how the user can resolve them.

### C.1 Special Error Traps in OPEN3

In all but one trap, PHAS3 must be exited to perform corrective action.

1. The file ASSIGN.CMP is written to the disk 1 device when INSTALL is executed. This file "tells" PHAS3 what the disk 2 device is. If ASSIGN.CMP can't be found on the disk 1 device, the user is returned to DOS. INSTALL must be carried out before starting PHAS3.

2. The file PROMPT.OPE is on the disk 2 device. If OPEN3 cannot find PROMPT.OPE on the disk 2 device, the generic message above is issued with error number of 53 at program line 620. In this case, the user must add PROMPT.OPE to the disk 2 device contents before proceeding further.

3. There are two other fatal error situations that are trapped in OPEN3.

- a. If the disk 2 device is a disk or diskette and is not in the correct drive, PHAS3 issues an error message. The user can insert the absent item.

- c. If both devices are on a hard disk and OPEN3 can't find the subdirectory specified for the disk 2 device, PHAS3 issues an error message and returns the user to DOS. This error is most likely caused by either failure to create the disk 2 device subdirectory or its incorrect designation in INSTALL.

### C.2 Missing File Error Traps

The traps discussed here all have error number 53.

OPEN3 at line 2970: An .OPE file is missing from the disk 1 device. This error occurs only in the program explanation routine. Check the .OPE files in the disk 1 device directory against those in Table 2 and add the missing file to the disk 1 device.

PATWAY3 at line 200: PATPMP.SCN is not on the disk 1 device. Add file to device; neither PATWAY3 or COMP3 operate without it.

PATWAY3 at line 880: All .PXX files for a specific environmental medium should be on the 2 device. As a minimum, the supplied file DEFL<pxx>.<pxx> must be on the device or scenarios dealing with the ".pxx" source medium cannot be developed. Add missing file(s) to the disk 2 device.

PTSED3 at line 2950, PTTOP3 at line 3000, and PTWAT3 at line 2910: A .SCN file is not on the disk 1 device. Check the .SCN files on the disk 1 device directory against those in Table 2 and add the missing file to the disk 1 device.

PTLD3 or PTLL3 at line 2912: A .CMP file is not on the disk 1 device. Check the .CMP files on the disk 1 device directory against those in Table 2 and add the missing file to the disk 1 device. A missing .CMP file may also disrupt CRDES3 operations.

PTLD3 or PTLL3 at line 3100: A .NCI file is not on the disk 1 device. Check the .NCI files on the disk 1 device directory against those in Table 2 and add the missing file to the disk 1 device.

NOCH3 at line 2100: A .NCI file is not on the disk 1 device. Resolve as discussed with PTLD3 or PTLL3.

CONTS or CONWS at line 9900: The file CONTTALK.CMP is missing. This file should be placed on the disk 1 device at the user's earliest convenience. The file provides on-line information about option selections that is discussed in Section 9.2. In this case, PHAS3 does not "crash"; after the error trap message, the option selection prompt will appear.

CRDES at line 9010: The specified .CMP file is not on the disk 1 device. In this case, the user is returned to the program from which CRDES3 was accessed; see Section 10.1. The user must add the .CMP file cited to the disk 1 device. The associated subroutine cannot be performed until this is done. A missing .CMP file may also cause a "crash" in PTLD3 or PTLL3.

CRD013 at line 9010: The specified .CMP file is not on the disk 1 device. There are three files whose absence can cause this error: MILLERM.CMP, VAPMENU.CMP and VPTABLE.CMP. In this situation, PHAS3 returns the user to CRDES3 at the "CRDES3 Central Processor" prompt (see Section 10.1). Until MILLERM.CMP is on the disk 1 device, the Miller Boiling Point Method can't be used. Until VAPMENU.CMP is on the disk 1 device, the vapor pressure subroutine can't be used. Until VPTABLE.CMP is on the disk 1 device, vapor pressure estimation method 2 or 5 can't be used. Add the missing file to the disk 1 device.

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